

**A Theoretical Study of Pyrolysis of JP-10 (*exo*-Tetrahydrodicyclopentadiene) and
its Primary and Secondary Unimolecular Decomposition Products**

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SUPPORTING INFORMATION

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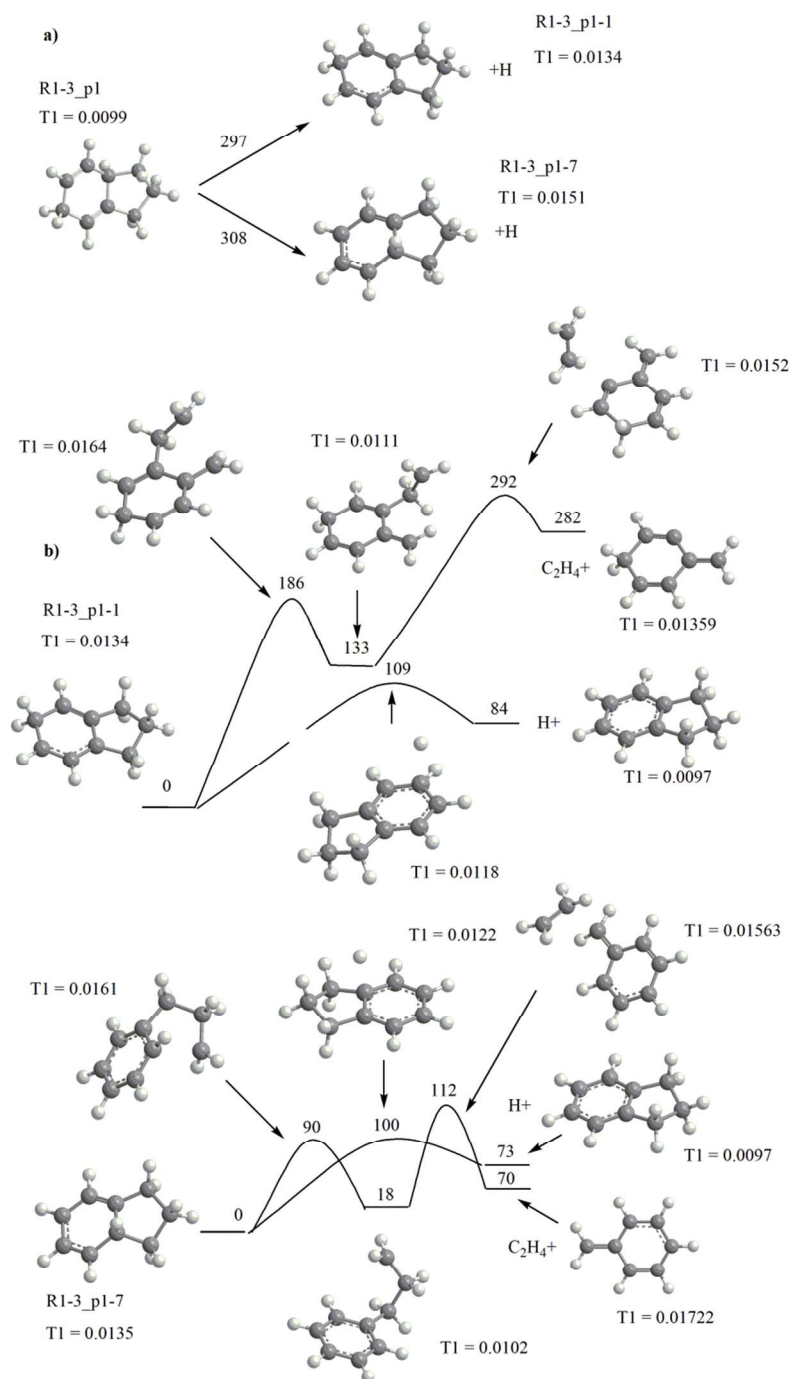


Figure S1. PESs for primary and secondary dissociation channels of C₉H₁₂ (R1-3_p1) with T1 diagnostics included. a) initial C-H bond cleavages, the numbers next to arrows show reaction endothermicities in in kJ mol⁻¹; b) PES for secondary dissociation channels of C₉H₁₂ (R1-3_p1), all relative energies are shown in kJ/mol.

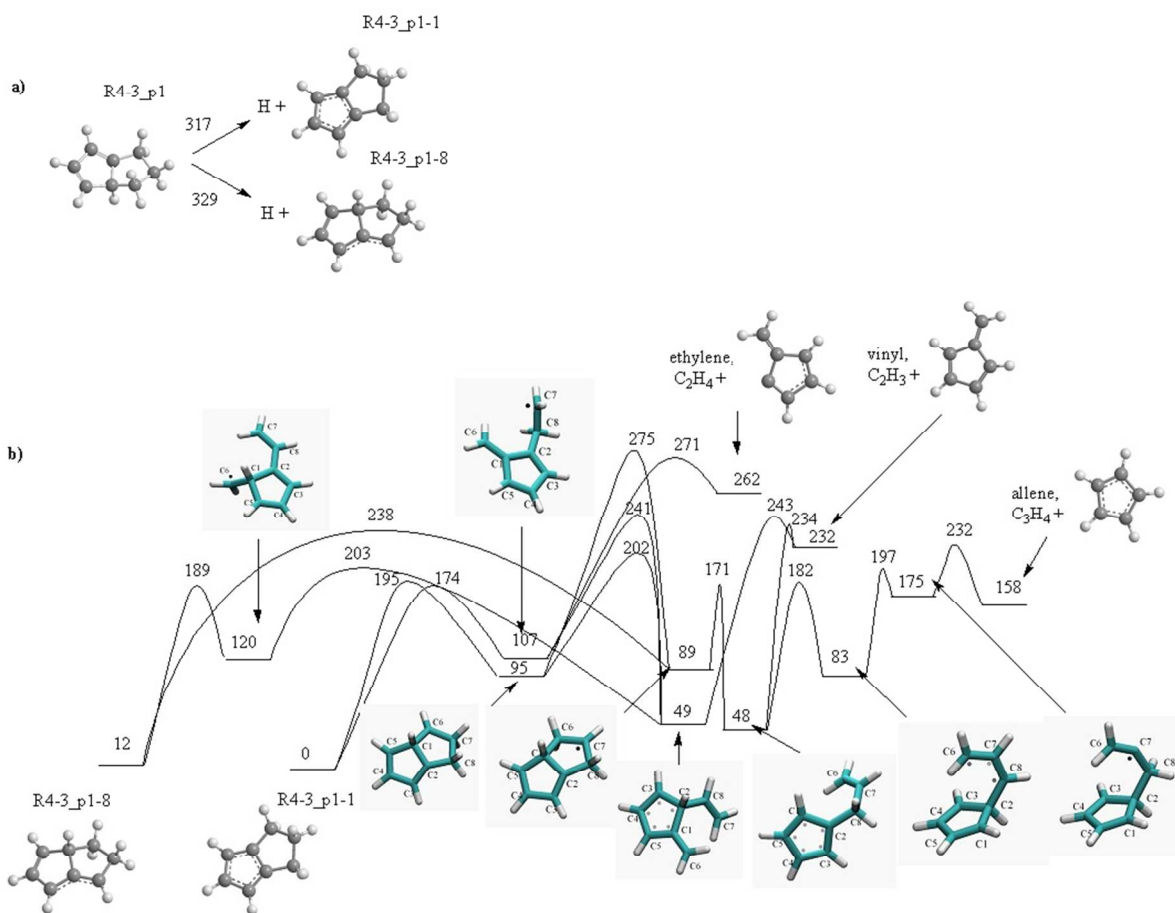


Figure S2. PESs for primary and secondary dissociation channels of C_8H_{10} (R4-3_p1): a) initial C-H bond cleavages, the numbers next to arrows show reaction endothermicities in kJ mol^{-1} ; b) PES for secondary dissociation channels of C_8H_{10} (R4-3_p1), all relative energies are shown in kJ/mol .

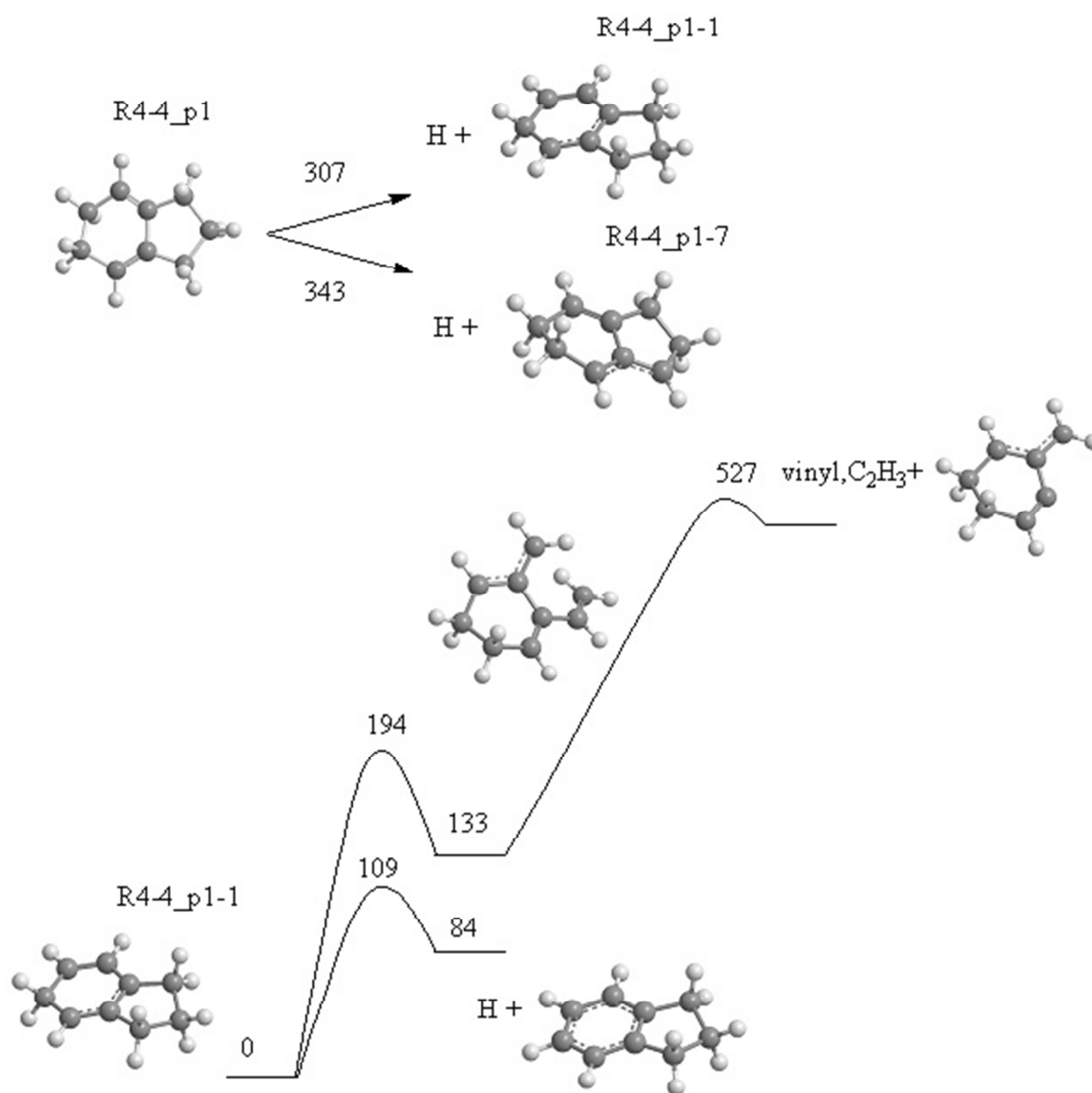


Figure S3. PESs for primary and secondary dissociation channels of C_9H_{12} (R4-4_p1): a) initial C-H bond cleavages, the numbers next to arrows show reaction endothermicities in kJ mol^{-1} ; b) PES for secondary dissociation channels of C_9H_{12} (R4-4_p1), all relative energies are shown in kJ/mol .

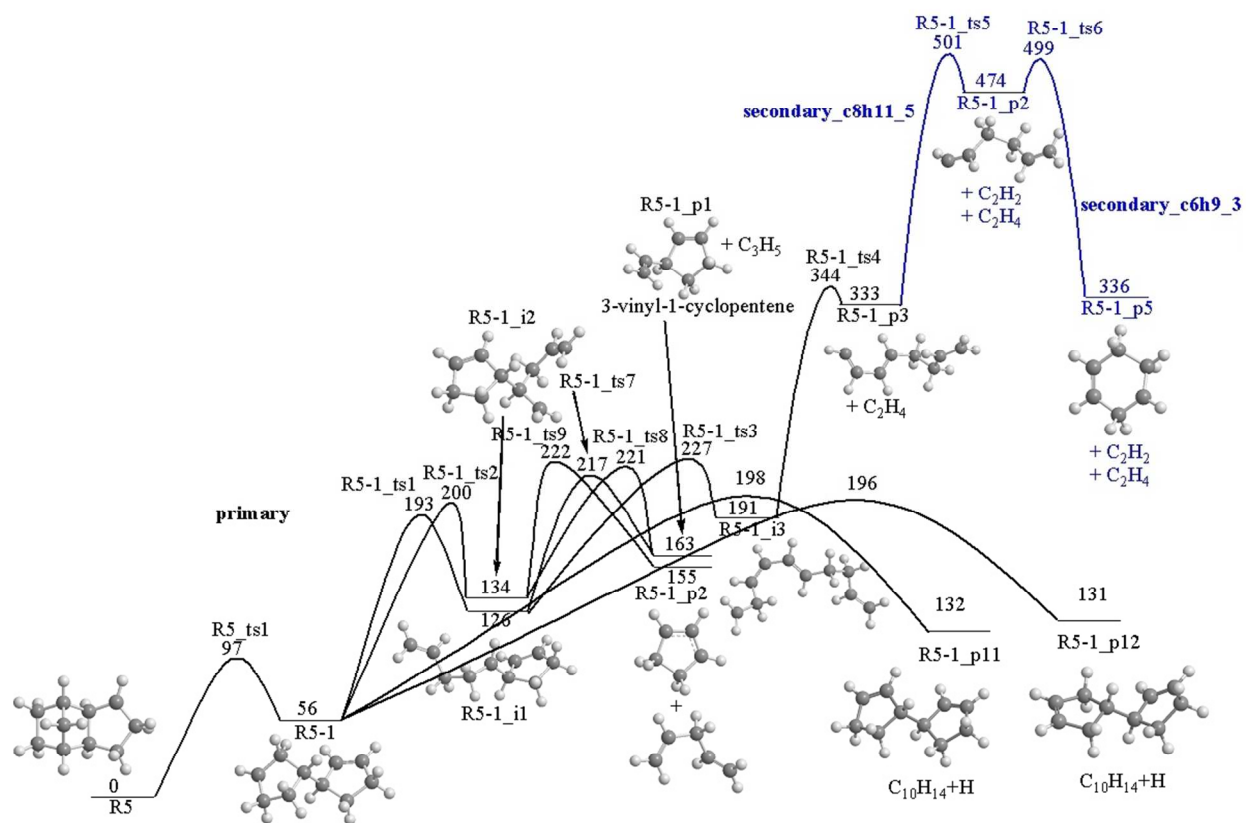


Figure S4. Potential energy diagram for decomposition of R5-1. All relative energies are given in kJ/ mol⁻¹.

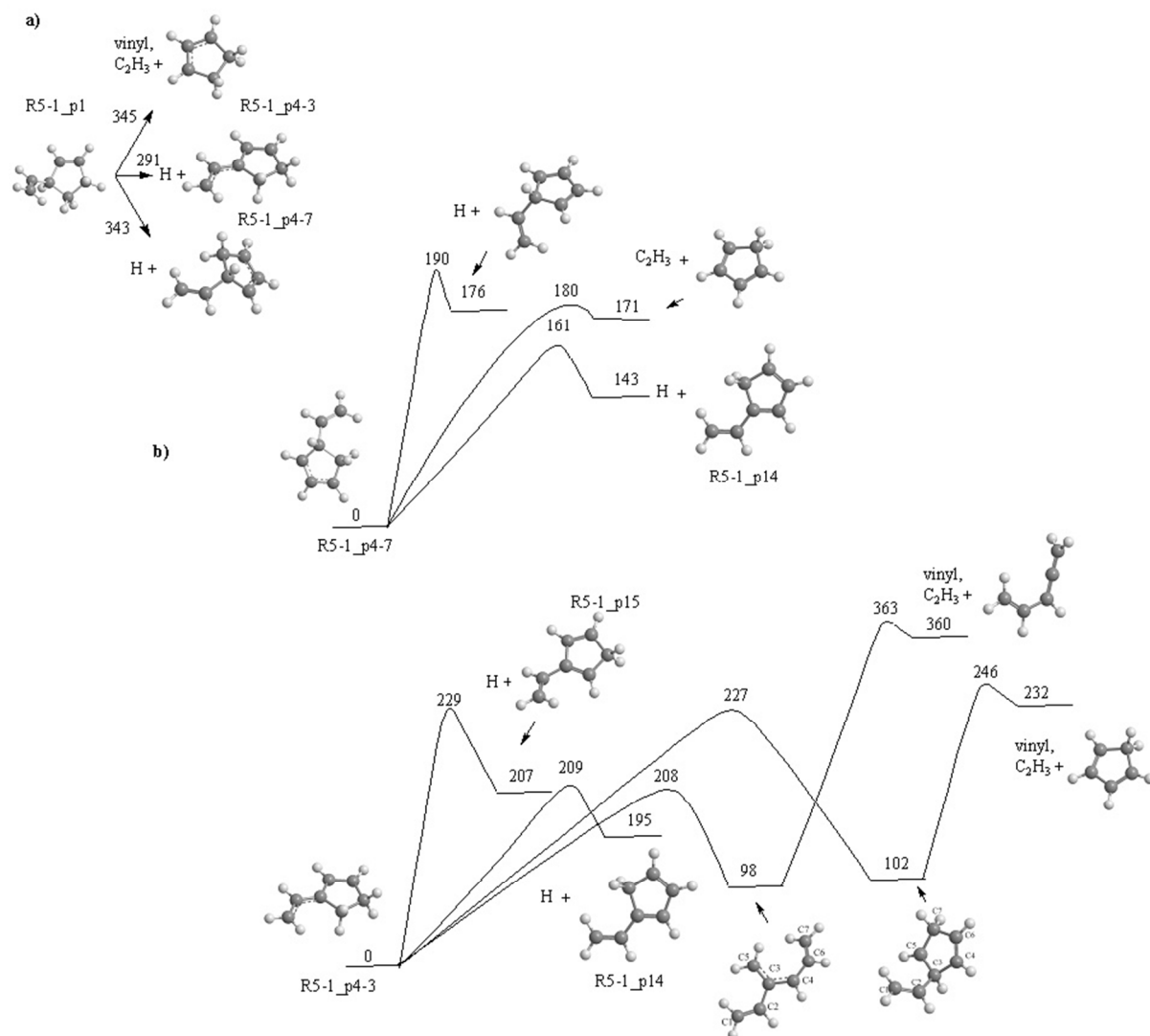


Figure S5. PESs for the dissociation channels of C_7H_{10} (R5-1_p1): a) initial C-H bond cleavages, the numbers next to arrows show reaction endothermicities in in kJ mol^{-1} ; b) PES for secondary dissociation channels of C_7H_{10} (R5-1_p1), all relative energies are shown in kJ/mol .

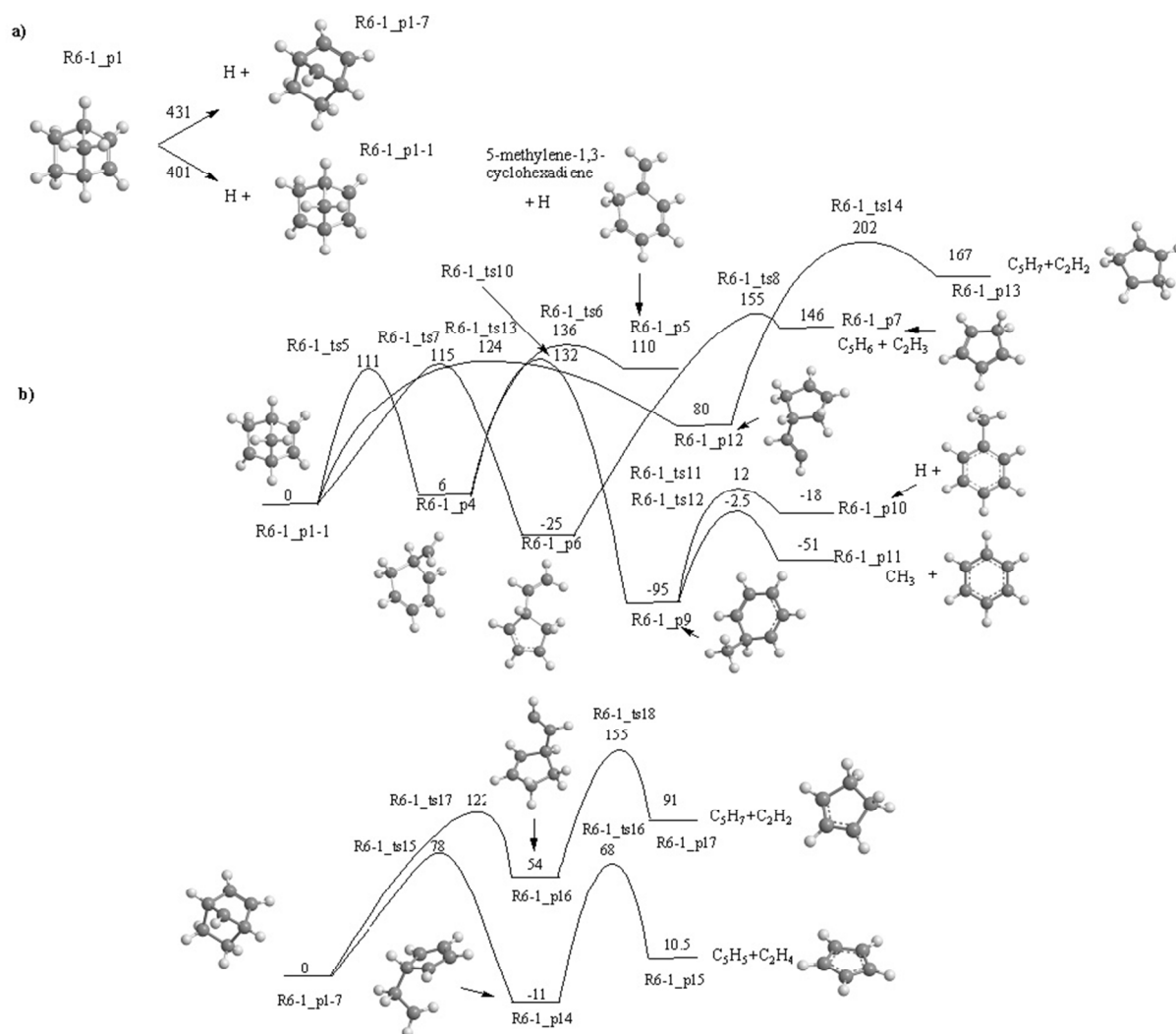


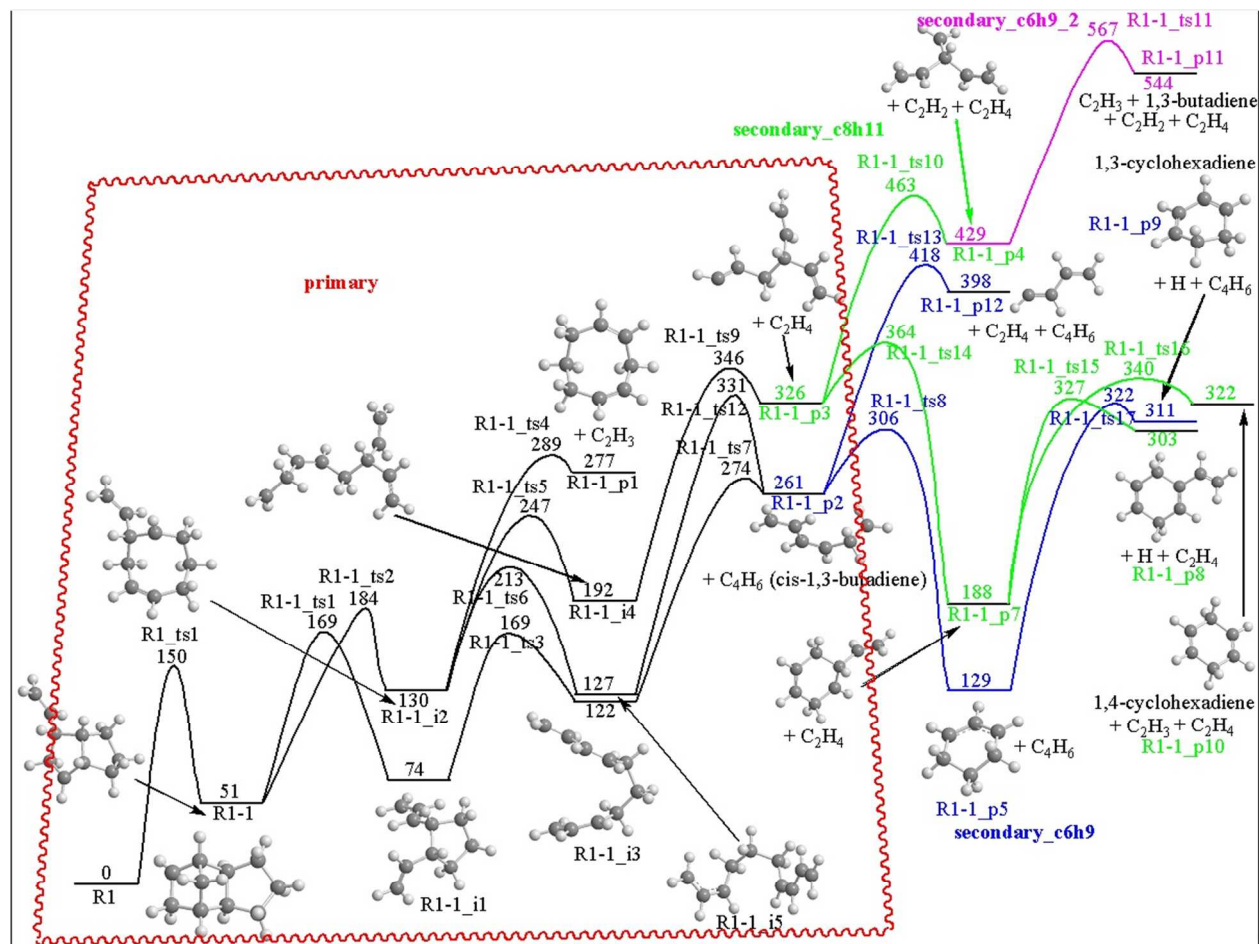
Figure S6. PESs for the dissociation channels of C_7H_{10} (R6-1_p1): a) initial C-H bond cleavages, the numbers next to arrows show reaction endothermicities in kJ mol^{-1} ; b) PES for secondary dissociation channels of C_7H_{10} (R6-1_p1), all relative energies are shown in kJ/mol .

Table S1. The experimentals versus the calculated (1500 K) branching ratios for the products of the JP-10 pyrolysis.

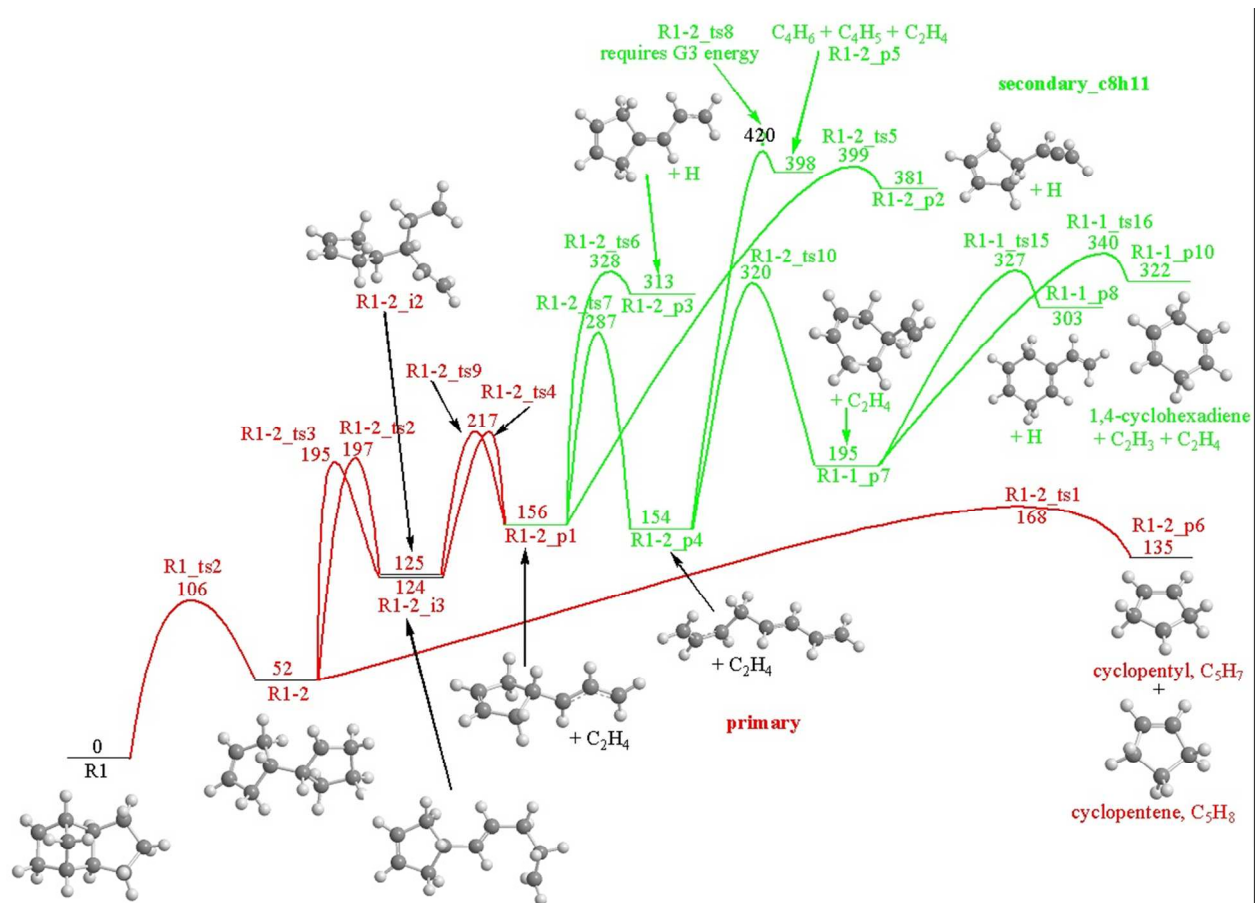
		calculated	experimental (ALS)
Methyl	CH ₃	2.02	2.73 (-0.61, +0.64)
Acetylene	C ₂ H ₂	2.40	0.54 (-0.12, +0.13)
Vinyl	C ₂ H ₃	1.43	0.38 (-0.20, +0.42)
Ethylene	C ₂ H ₄	12.12	24.59 (-5.21, +5.35)
Ethyl	C ₂ H ₅	0.12	2.37 (-0.53, +0.55)
Propargyl	C ₃ H ₃	0.02	0.26 (-0.06, +0.07)
Allene	C ₃ H ₄	0.00	2.50 (-0.60, +0.66)
Methylacetylene	C ₃ H ₄	0.00	0.86 (-0.20, +0.22)
Allyl	C ₃ H ₅	24.50	12.95 (-3.11, +3.37)
Propene	C ₃ H ₆	0.00	0.83 (-0.19, +0.20)
Diacetylene	C ₄ H ₂	0.00	-
1,2,3-Butatriene	C ₄ H ₄	0.25	0.05 (-0.04, +0.10)
Vinylacetylene	C ₄ H ₄	0.46	0.09 (-0.02, +0.02)
1,3-Butadiene	C ₄ H ₆	1.70	2.49 (-0.53, +0.55)
1-Butene	C ₄ H ₈	0.00	0.09 (-0.03, +0.03)
2-Butene	C ₄ H ₈	0.00	0.03 (-0.01, +0.02)
Ethynylallene	C ₅ H ₄	0.00	-
Cyclopentadienyl	C ₅ H ₅	1.07	3.09 (-1.59, +3.27)
Cyclopentadiene	C ₅ H ₆	20.58	19.91 (-4.39, +4.60)
Cyclopentenyl	C ₅ H ₇	16.05	-
1,3-Pentadiene	C ₅ H ₈	0.64	0.47 (-0.13, +0.15)
Cyclopentene	C ₅ H ₈	5.69	2.93 (-0.66, +0.70)
Fulvene	C ₆ H ₆	0.64	13.28 (-6.89, +14.28)
Benzene	C ₆ H ₆	2.22	4.46 (-0.97, +1.01)
1,3-Cyclohexadiene	C ₆ H ₈	0.56	0.20 (-0.04, +0.05)
1,4-Cyclohexadiene	C ₆ H ₈	0.13	0.32 (-0.08, +0.09)
Cyclohexene	C ₆ H ₁₀	0.01	0.14 (-0.05, +0.06)
Fulvenallenyl	C ₇ H ₅	0.00	-
Fulvenallene	C ₇ H ₆	2.76	0.04 (-0.02, +0.04)
5-Methylene-1,3-cyclohexadiene	C ₇ H ₈	4.06	0.73 (-0.38, +0.80)
Toluene	C ₇ H ₈	0.17	0.40 (-0.22, +0.46)
Phenylacetylene	C ₈ H ₆	0.00	-
Benzocyclobutadiene	C ₈ H ₆	0.00	-
o-Xylylene	C ₈ H ₈	0.24	0.03 (-0.02, +0.03)
Styrene	C ₈ H ₈	0.03	0.11 (-0.03, +0.03)
1,3,5-Cyclooctatriene	C ₈ H ₁₀	0.00	0.19 (-0.10, +0.20)
o-Xylene	C ₈ H ₁₀	0.00	0.27 (-0.07, +0.07)
Indene	C ₉ H ₈	0.00	-
Indane	C ₉ H ₁₀	0.14	0.06 (-0.01, +0.02)

Cartesian coordinates and vibrational frequencies of stationary points in R1 channel

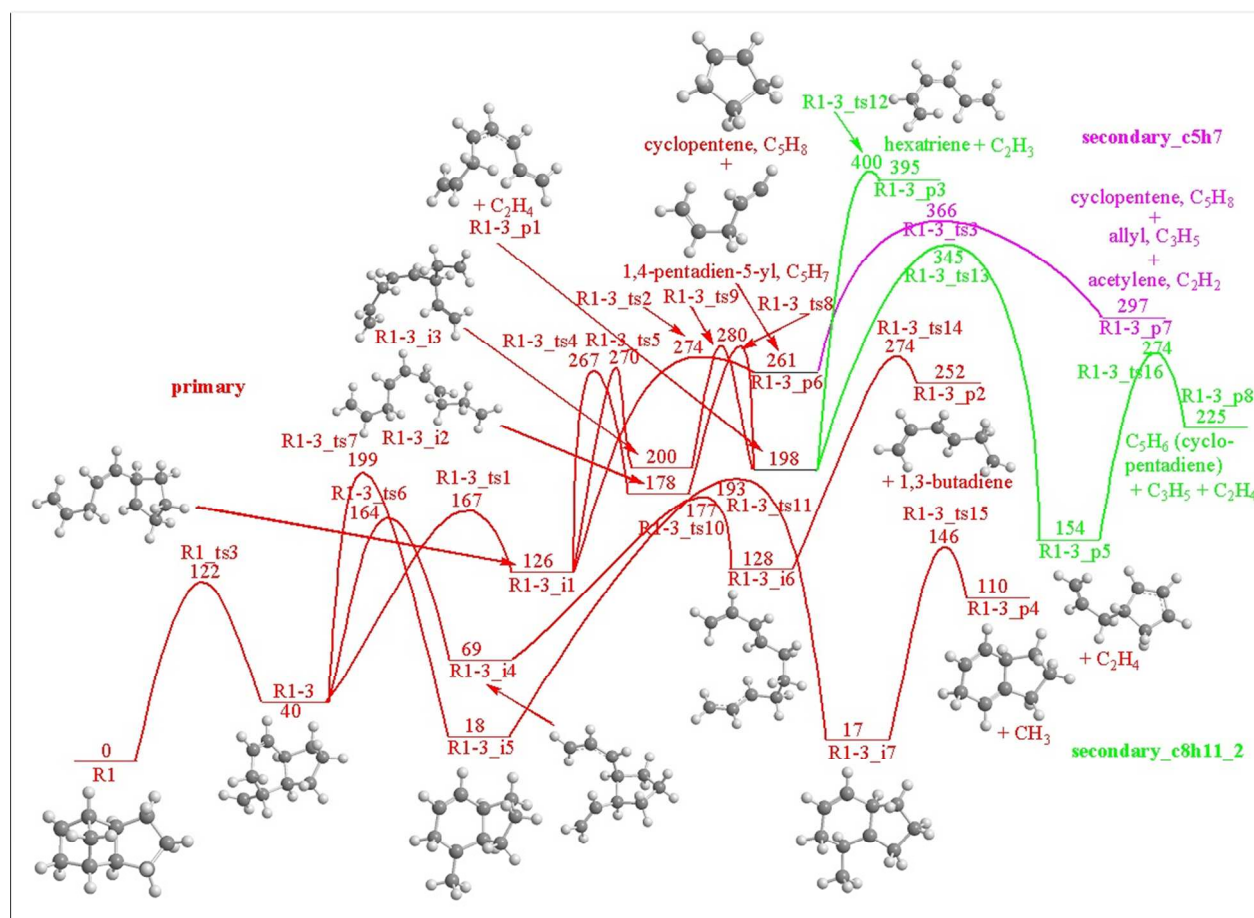
Please refer to the following schemes for the notation of stationary points involved in R1 channel. Cartesian coordinates and vibrational frequencies of the stationary points are given below in the form of the corresponding fragments of the MESS input file.



Scheme S1. R1-1 PES.



Scheme S2. R1-2 PES.



Scheme S3. R1-3 PES.

R1_primary

```
!-----c10h15_R1-----
Well      R1
Species
RRHO
Geometry[angstrom]  25
C   -0.7756288993    0.2137117194    2.1424312222
C   -0.1157449135   -1.1412134357    2.1989622427
C    0.8682271677   -1.0539006228    1.0013109409
C    0.0358194708   -1.0683382237   -0.3066299928
C   -0.656130578    0.3503222848   -0.3125549994
C   -0.137742638    0.9845483437    1.0216009805
C    1.3065855856    0.4250762128    1.0845646293
C    0.8385293648   -1.1468938818   -1.6256920536
C   -0.2082084592    1.0348851524   -1.625346132
C    0.1610960871   -0.1297511748   -2.5611256843
H   -1.7137380248    0.4696414985    2.6188978185
H   -0.8208410458   -1.9774465808    2.1060293313
```

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H  0.4279051278   -1.2980926511   3.1430565426
H  1.6678003721   -1.7967574981   1.0266359128
H  -0.7052881959   -1.8721616982   -0.2778249611
H  -1.7452288626    0.2651935826   -0.292502946
H  -0.2517952653    2.0690694685   1.0680182192
H  1.9388492049    0.7429809169   0.2526580846
H  1.8136658746    0.6705593447   2.0209171764
H  0.8582266617   -2.1581053105   -2.0401176677
H  1.8803096779   -0.8522836802   -1.4558455234
H  0.6736692215    1.6608205951   -1.4495254512
H  -0.9835173322    1.684772608    -2.0389501882
H  -0.7495007525   -0.5659008177   -2.9878030849
H  0.7965491506    0.174780848    -3.3973994164
Core RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
148.2320           174.2653           267.6776
297.5737           317.0214           364.7048
433.3435           496.6229           547.7499
565.0848           671.0031           744.5008
763.3266           792.6544           860.9382
863.2533           889.2926           903.1325
906.6943           912.6670           932.4186
934.2306           954.6901           978.6127
995.8764           1008.4037          1031.8521
1039.4356           1050.0249          1068.8346
1119.7275           1143.2540          1155.1139
1184.4321           1192.8055          1209.3288
1231.8398           1249.7453          1268.1589
1278.9165           1297.6216          1303.6151
1315.1429           1323.3460          1334.0306
1341.6208           1342.9160          1357.0562
1366.4476           1472.0595          1492.6165
1495.8573           1505.5577          1519.1767
2962.3990           3004.7119          3017.1596
3022.0726           3025.3816          3035.9658
3049.3774           3052.4856          3067.6725
3072.7016           3078.6151          3080.5875
3083.7046           3093.3484          3191.0127
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----c10h15_R1-1-----
Well          R1-1
Species
RRHO
Geometry[angstrom]  25
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C	0.8313062638	-1.7933152969	0.5644499859
C	0.6441849821	-0.2457664598	0.4275053405
C	-0.632487957	0.0704008828	1.2646752701
C	-1.5281746657	-1.1797706641	1.0643351405
C	1.3479379718	-2.2652305225	-0.8153770736
C	0.5796819937	0.0193441216	-1.1104583774
C	0.5958942721	-1.361171193	-1.8021017204
H	-1.757632218	1.4884121214	-0.0041737466
H	-1.9199963535	3.3102523123	1.5821868853
H	-0.9946318402	2.3268919855	2.8435183264
H	-0.7984841193	-3.34164354	0.9638813016
H	1.5519721976	-2.0548455041	1.3526530951
H	1.4890869264	0.3007818863	0.8515689599
H	-0.3167948266	0.0776574798	2.3145942111
H	-2.2286291123	-1.3243088897	1.8949616176
H	-2.1557952043	-1.0583567664	0.1634613118
H	1.1778894258	-3.331486526	-0.9865450023
H	2.4276593417	-2.0877233165	-0.8846515644
H	1.4614727065	0.5925292751	-1.4105854233
H	-0.286171927	0.6137121001	-1.4074158337
H	-0.425531125	-1.7327827983	-1.9328947486
H	1.058110338	-1.3292952327	-2.7918421748

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 69

60.9864	78.7603	130.7936
205.2284	231.4586	275.5079
334.3562	370.4923	416.2140
440.8450	553.3813	601.0521
636.8259	678.9285	751.1181
790.0491	841.7393	857.2716
877.8216	905.7567	908.3346
944.0633	946.0846	960.9612
999.0808	1008.9883	1025.8840
1034.9348	1036.4941	1083.4006
1091.3388	1115.3799	1143.9983
1172.5135	1195.7165	1210.0303
1264.8822	1267.3733	1276.5814
1297.3778	1310.7822	1316.5790
1323.3663	1334.3983	1343.3607
1351.7891	1360.5501	1371.2523
1459.6232	1475.5570	1492.7006
1494.5363	1511.7541	1701.7599
2915.8033	2968.1911	3012.7641
3018.1251	3028.2780	3030.2350
3038.5876	3064.8501	3071.3962
3076.6109	3090.8039	3118.2284
3126.4570	3177.1774	3206.0973

ZeroEnergy[kcal/mol] 12.19

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ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----c10h15_R1-1_i1-----
Well      R1-1_i1
Species
RRHO
Geometry[angstrom]    25
C  -0.917953372    1.4683692825    0.5752614423
C  -2.1048143371    1.9740030725    1.0758110706
C   0.4648015552   -2.4368560656    1.6599784868
C   1.0443341754   -1.6656627165    0.5088004994
C   1.1344837385   -0.1107996744    0.7087541482
C  -0.1642679529    0.4772574168    1.1836944298
C  -0.5641895521   -3.2795389699    1.6218747874
C   0.3574419077   -1.7963672285   -0.8617193477
C   1.6074847731    0.3375028368   -0.6875078189
C   0.8862028882   -0.59853153   -1.6962872209
H  -0.5601639932    1.8877812265   -0.362002691
H  -2.6515520627    2.7497307355    0.5552215124
H  -2.5237712975    1.6062123595    2.0060869391
H   0.9740261059   -2.2870985605    2.6120915259
H   2.0870098838   -2.0006325488    0.3992462336
H   1.899734565    0.1055411078    1.4677382051
H  -0.545088676    0.06918101    2.1176334444
H  -0.8948445132   -3.8021737105    2.5125783494
H  -1.1117069991   -3.4846261557    0.7086954069
H  -0.725920719   -1.7170588136   -0.7366769428
H   0.5601238084   -2.7608698468   -1.33268198
H   2.6891337927    0.187225036   -0.7487805253
H   1.4309624155    1.3961914634   -0.8845758235
H   0.0634231636   -0.0851160168   -2.1985355385
H   1.5743027015   -0.9269727099   -2.4787795925
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]    69
34.8023              82.4031              95.6352
121.0354             145.9563             215.3446
252.2317             271.1184             350.0565
428.1587             474.2368             542.5885
553.9108             583.6756             683.4573
716.9528             760.1727             782.0072
801.6486             828.7474             860.6721
894.5864             935.5388             944.9695
964.1779             992.5184             996.7085
1016.0697            1034.5724            1045.0001
1054.6226            1091.3505            1140.4034
1163.0704            1206.0949            1209.2623
1236.4997            1271.0670            1277.9944

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1291.3536	1295.5885	1324.5750
1331.2375	1337.1587	1351.5648
1371.2018	1390.6499	1453.6730
1493.9037	1498.6582	1503.1547
1519.1659	1523.1199	1703.0449
2967.9510	2980.9895	3040.5389
3042.0667	3053.2992	3070.7059
3086.4602	3097.2914	3105.6071
3126.2082	3136.9503	3137.6042
3138.8295	3214.4351	3232.3336

ZeroEnergy[kcal/mol] 17.69

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h15_R1-1_i2-----

Well R1-1_i2

Species

RRHO

Geometry[angstrom] 25

C	1.8783194277	-0.4722332972	-0.5114452306
C	3.1289211374	-0.2320925683	-0.1252752549
C	-1.3968893144	1.6075652687	-0.3928313141
C	-2.5767498419	1.0280298263	-0.1573332676
C	-0.1894993012	-0.9321403364	0.7660118753
C	0.6382778185	0.1407542262	0.1070986904
C	-0.1327307076	0.9919558016	-0.9432308687
C	-3.0735900853	-0.3745447826	-0.4111957412
C	-1.0515810223	-1.9404742614	0.0691665434
C	-2.107431437	-1.4413665822	-0.9447699599
H	1.699270788	-1.1695067538	-1.3290762889
H	3.9756056327	-0.7119074207	-0.603794105
H	3.3508387055	0.4546702246	0.6864036977
H	-1.3099088657	2.6539565742	-0.1081802406
H	-3.3426367771	1.6666081666	0.2818275045
H	0.0632506665	-1.1487178913	1.7992982451
H	0.9702409491	0.8235523471	0.8980278836
H	0.538796493	1.7880739256	-1.276708121
H	-0.3333412113	0.3834817294	-1.826370079
H	-3.9192935696	-0.296439655	-1.1088688773
H	-3.5211130127	-0.742114977	0.52345619
H	-1.5737397093	-2.5181431176	0.8405939262
H	-0.4187422953	-2.6780883527	-0.4562800072
H	-1.6339212271	-1.094614882	-1.8649924131
H	-2.7038332408	-2.3129032121	-1.236967787

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 69

47.4511	84.8985	128.8051
176.9190	226.4254	259.7946

277.6448	314.8924	336.2120
390.3483	401.5950	502.2827
513.9495	631.9425	673.8071
686.9282	709.4737	774.7353
807.6173	854.7884	882.3514
912.6253	933.8806	937.0386
988.9004	1004.7770	1014.1257
1015.3671	1030.0600	1074.4191
1095.4671	1133.7579	1161.1937
1183.2928	1202.8712	1244.8179
1281.9500	1292.5008	1303.8726
1321.0243	1336.4770	1353.5505
1372.4587	1386.6228	1399.0145
1402.7129	1434.2896	1448.3238
1467.1716	1475.3315	1489.5197
1523.1705	1687.7897	1720.5489
2916.8625	2983.9597	2999.3109
3015.5033	3023.1823	3031.2707
3046.9275	3074.0285	3096.7183
3103.1657	3114.3581	3125.1494
3132.5445	3151.8500	3204.9354

ZeroEnergy[kcal/mol] 31.07

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h15_R1-1_i3-----

Well R1-1_i3

Species

RRHO

Geometry[angstrom] 25

C	0.2073683693	2.3470353656	1.4017103954
C	-0.2287241822	2.8761684661	2.5511624024
C	0.6248354377	-2.205018199	1.2386949071
C	1.3685122827	-1.7815180848	0.140964748
C	2.0798320835	1.3503299208	0.0669084289
C	1.5664655756	1.8731240546	1.1928065526
C	-0.7481312648	-2.30540155	1.3282957077
C	0.8206093638	-1.3729910717	-1.1916224841
C	1.4039458948	1.1617864809	-1.2619294932
C	1.591322031	-0.2352535723	-1.8876803623
H	-0.4889925983	2.2631924172	0.5723427881
H	-1.2504400904	3.2162994047	2.6698331599
H	0.426595912	2.9831653551	3.4101393669
H	1.1955414006	-2.4875531132	2.1208490196
H	2.4510311254	-1.7931122748	0.2327046506
H	3.1265050982	1.0518231758	0.0899953718
H	2.2239970276	1.9570520611	2.0556141473
H	-1.2205106186	-2.6446959861	2.2412292081
H	-1.4026815019	-2.0500041115	0.5039040246
H	-0.2343748918	-1.0926464589	-1.105886799

```

H  0.8409371793   -2.2466586786   -1.8617342534
H  1.8267675544    1.8955677546   -1.9623523919
H  0.3355949781    1.3868233288   -1.1980183368
H  1.263934257    -0.1864809596   -2.931478
H  2.659913577    -0.482624725   -1.9153587584
Core RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
22.8306           33.7919           41.0060
109.6537          126.5372          184.2527
213.2750          254.9481          303.5117
308.7254          374.7601          401.1417
453.0516          545.1521          581.4515
628.2175          661.5981          685.4810
788.2412          791.1576          809.7307
860.3024          904.4193          920.0217
928.3351          963.2083          987.6826
991.3638          1006.0667         1034.7710
1039.3082          1070.6292         1082.9672
1138.4053          1196.3495         1204.5038
1236.5656          1244.1895         1274.0328
1292.3606          1321.6217         1345.2967
1362.6484          1380.2291         1405.0603
1437.1208          1465.9863         1470.8339
1474.3971          1481.4308         1494.6483
1529.2413          1653.5144         1703.2715
2962.0534          2990.1816         3011.1108
3041.8102          3050.8712         3065.7856
3113.8610          3124.0518         3129.8722
3136.8459          3145.0349         3151.2610
3152.1407          3218.3338         3234.6121
ZeroEnergy[kcal/mol] 29.16
ElectronicLevels[1/cm] 1
0  2
End
End
!-----
!-----c10h15_R1-1_i4-----
Well      R1-1_i4
Species
RRHO
Geometry[angstrom]  25
C  1.8878371889    1.2316433319    0.6163546961
C  1.9575008315    2.0489118646    1.6627842193
C  -0.9726857828    1.2353030854    -0.5239806277
C  -2.3036917523    1.1518497856    -0.4547371087
C  1.8871211508    -1.2231864084    0.4656819592
C  1.0025521672    0.0075761923    0.514686547
C  0.0133967234    0.1097933275    -0.6727436005
C  -3.1658301445    -0.0850853509    -0.5239992917
C  2.0108141979    -2.0904768126    -0.53543853

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C	-4.0674691906	-0.1014114049	-1.716882544
H	2.5193779776	1.4164209981	-0.2518816696
H	2.6262803587	2.9024248691	1.673884085
H	1.3461678475	1.8945584118	2.5468390256
H	-0.5316327622	2.2270171315	-0.456689268
H	-2.8616357498	2.0807803125	-0.3550274802
H	2.492436735	-1.3659544798	1.3588719534
H	0.4122981542	-0.0505764195	1.4385239839
H	0.5909642266	0.2595767011	-1.5946115784
H	-0.500623468	-0.8474805826	-0.7808146
H	-3.7745805515	-0.1487741344	0.3878704054
H	-2.5381428516	-0.9893440209	-0.5132960715
H	2.6916447034	-2.9312040504	-0.4629985439
H	1.4473069085	-2.0048926742	-1.4576167594
H	-3.7233019116	0.2875200857	-2.6674297468
H	-5.0254070063	-0.6060317584	-1.6852364547

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 69

26.6856	50.0097	73.9939
82.6033	105.6875	123.6972
149.4891	225.0871	254.2787
312.2192	327.2989	361.9401
415.8437	474.7021	516.4537
544.9960	589.7401	646.0965
697.5261	756.7957	790.1357
851.2201	934.7377	941.4607
947.5904	949.6428	977.5034
1001.4735	1016.6898	1035.5066
1040.1835	1044.7919	1070.5694
1090.4598	1130.1915	1140.8632
1206.9752	1242.7723	1283.8349
1295.9957	1315.4720	1320.6787
1328.9203	1338.3396	1358.7600
1433.5238	1447.5036	1451.7190
1457.2934	1462.8609	1491.0481
1691.9107	1704.0499	1716.9446
2961.9839	2997.3081	3005.2290
3010.4390	3080.2400	3115.7819
3119.1281	3124.2264	3128.0863
3134.7276	3140.2713	3144.4777
3208.7259	3215.6065	3240.5853

ZeroEnergy[kcal/mol] 45.89

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h15_R1-1_i5-----

Well R1-1_i5

Species

RRHO

Geometry[angstrom] 25

C	2.1600587743	-1.046584656	-0.328932217
C	3.4593328972	-0.7376743397	-0.4155355457
C	-2.6157752189	2.2091918377	-1.0719628594
C	-2.7480834823	1.0876012178	-0.2569311907
C	-0.0978848042	-0.5969847016	0.6621022332
C	1.2161102809	-0.3484972214	0.531076852
C	-2.7323441285	2.25177323	-2.4462118917
C	-3.0418088339	-0.3008583662	-0.7443907356
C	-0.8993882817	-1.6533627902	-0.047432208
C	-1.8133031559	-1.1392113276	-1.1834278607
H	1.78050105	-1.8632386681	-0.9366806454
H	4.131081944	-1.2810522734	-1.0692021533
H	3.8896045305	0.0719383722	0.1659564697
H	-2.3970534375	3.1477644242	-0.567078363
H	-2.6318073507	1.2315623548	0.8121443503
H	-0.6517529609	0.0323029773	1.3525069847
H	1.6394174461	0.4609842158	1.1222799803
H	-2.6124921457	3.1826536114	-2.9855288588
H	-2.9489710165	1.3686391186	-3.0350566363
H	-3.7233790379	-0.2450672179	-1.6004634819
H	-3.5767541235	-0.8543675264	0.036266038
H	-1.5243800116	-2.1773778779	0.6877664827
H	-0.2322368104	-2.4091229585	-0.4697670495
H	-1.2154949654	-0.5602823686	-1.8938155633
H	-2.1903561574	-2.0149020664	-1.7243421306

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 69

17.1307	36.7820	48.5488
109.6680	130.1631	182.7012
204.1198	246.4984	283.5353
343.9372	393.5134	419.4854
491.8977	543.7924	576.3292
612.5621	673.3913	716.5519
781.1461	796.1688	810.2337
849.0686	884.4879	916.9627
930.1857	964.9426	991.6204
995.3975	1004.8905	1040.4901
1043.4880	1052.0909	1084.7391
1145.3690	1187.4790	1203.7059
1238.3382	1246.8474	1282.0796
1302.1811	1325.5257	1347.7966
1356.2327	1370.9033	1405.6309
1432.1202	1468.5990	1472.9791
1487.8141	1492.0721	1497.8582
1528.4076	1653.0495	1703.5688
3002.1058	3008.4473	3017.4026
3044.6927	3066.3646	3071.0715
3122.9106	3126.3319	3130.7239

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3146.1927          3147.4541          3154.8347
3164.1329          3217.8285          3235.2607
ZeroEnergy[kcal/mol] 30.35
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R1-2-----
Well          R1-2
Species
RRHO
Geometry[angstrom] 25
C -3.0903720466 -0.4220044063 -0.1545394662
C -2.7919382525 0.7689391642 -0.6700644833
C -1.3749465408 1.1869429793 -0.3589485168
C -0.9245360847 0.160306626 0.7202812229
C -1.9272217796 -1.0238091536 0.5965647685
C 0.5642721043 -0.2451080765 0.6943409035
C 1.0746761525 -0.9682927246 -0.5799270456
C 2.5888365272 -0.6868580788 -0.5977604756
C 2.7132466417 0.7582667522 -0.0609962033
C 1.5249268123 0.9000006106 0.8368775902
H -4.0378107382 -0.9345192519 -0.2803802285
H -3.4619329478 1.369035191 -1.2760204932
H -1.3049060066 2.2171379315 0.0039895748
H -0.7533355412 1.1415508378 -1.2625071173
H -1.1068516676 0.6290234448 1.6940307505
H -1.5022440044 -1.8650493247 0.0333382037
H -2.2115715836 -1.4233040517 1.575911122
H 0.7043261881 -0.9380238563 1.5456246235
H 0.6073377945 -0.5345661858 -1.4702716502
H 0.8462017614 -2.0364643535 -0.5818499794
H 3.034552964 -0.817256274 -1.5867513688
H 3.0998464998 -1.3747520956 0.0840889679
H 2.6751641184 1.4824861105 -0.8920371672
H 3.6675339912 0.9427372404 0.4476690851
H 1.3867556385 1.7135769451 1.5393253827
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
52.0437          73.4372          103.3104
196.5991          208.3170          271.9171
338.9368          371.3961          392.2582
528.2648          554.7749          618.1886
690.2705          709.5431          781.1224
805.7368          841.4348          873.8694
888.7616          912.3300          921.5193
939.0633          956.1083          976.0668
976.3673          1002.4595          1019.9707
1035.6056          1055.5550          1075.5796

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1109.8448	1122.6831	1136.6693
1160.3316	1195.6454	1214.1150
1227.9678	1270.9833	1288.9044
1292.5657	1299.4864	1308.2789
1329.3254	1334.8087	1339.2622
1363.6538	1373.0770	1388.1743
1471.8285	1486.2885	1494.7928
1496.8346	1507.4665	1682.2044
2884.7458	2932.1485	3000.9768
3003.1516	3007.8863	3011.9320
3029.8646	3032.6793	3039.3675
3048.9043	3075.1650	3084.0264
3161.6345	3179.9988	3186.5930

ZeroEnergy[kcal/mol] 12.43

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h15_R1-2_i2-----

Well R1-2_i2

Species

RRHO

Geometry[angstrom] 25

C	2.850409	-0.345915	-0.730303
C	2.994518	0.269548	0.441401
C	1.68426	0.41011	1.17621
C	0.71483	-0.503998	0.370777
C	1.416537	-0.732981	-1.001597
C	-0.758981	-0.02049	0.329384
C	-0.953954	1.315077	-0.434493
C	-2.301089	1.922331	-0.249695
C	-2.587736	-1.758103	0.430873
C	-1.652454	-1.092741	-0.241567
H	3.650164	-0.527151	-1.439878
H	3.929003	0.66256	0.826346
H	1.360743	1.458971	1.18755
H	1.748796	0.101304	2.224897
H	0.702383	-1.471864	0.881468
H	1.315666	-1.767948	-1.343647
H	0.998118	-0.105422	-1.798949
H	-1.064718	0.149566	1.369261
H	-0.767808	1.136281	-1.508093
H	-0.18326	2.034473	-0.134511
H	-2.457748	2.978569	-0.431657
H	-3.169464	1.300747	-0.070176
H	-3.188459	-2.529024	-0.03912
H	-2.785387	-1.556569	1.479735
H	-1.494362	-1.327338	-1.294218

Core RigidRotor

SymmetryFactor 1.0

End

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Frequencies[1/cm]  69
47.6775           70.2015           87.8467
99.7900           140.4561          193.0901
234.0200          286.0188          313.8756
382.9787          391.5815          435.0469
492.9450          535.2117          617.5661
706.9585          734.2011          761.7995
783.3929          833.7175          919.4513
927.0821          939.9164          947.0708
956.9269          976.9504          977.5816
1017.8657         1037.0312         1045.2061
1068.9976         1075.3306         1118.5807
1130.6708         1138.0221         1167.2074
1207.9956         1226.6872         1289.5304
1301.1345         1305.6124         1322.7737
1331.7778         1341.0512         1359.8861
1373.0430         1387.8439         1454.4829
1458.7464         1466.5046         1491.2220
1497.9084         1683.6926         1701.0750
2921.7375         3001.8025         3004.5814
3009.1389         3023.8825         3027.1490
3040.2627         3051.6969         3108.0016
3123.7562         3137.2282         3163.4778
3188.2545         3204.7296         3239.9141
ZeroEnergy[kcal/mol] 29.88
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R1-2_i3-----
Well          R1-2_i3
Species
RRHO
Geometry[angstrom]  25
C  -3.0781382425  -0.2300736391  -0.0370486928
C  -2.9132234902  1.0676074664  0.2127978278
C  -1.4620498418  1.4152424648  0.4564812172
C  -0.8130750768  0.0312936401  0.7124981862
C  -1.7675719154  -0.9793788072  0.0043020321
C  0.6377492991  -0.1490226738  0.3582511169
C  3.0138161602  -1.7890268038  -1.2512841007
C  3.5208024899  -0.8084442147  -0.2503833023
C  2.9464653172  0.6084245742  -0.3909943893
C  1.4863963708  0.7897861539  -0.0585105309
H  -4.0215835877  -0.7029867191  -0.2856801697
H  -3.7019720505  1.8113772465  0.1975726587
H  -1.3132784403  2.1068663096  1.2913264316
H  -1.0417453413  1.9009884828  -0.4342854893
H  -0.9149449213  -0.168357011  1.7885078771
H  -1.4192542955  -1.2057879131  -1.0123982535
H  -1.8273489256  -1.934244306  0.5363742193

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H  1.0014776756   -1.1687595595   0.4719006579
H  2.5868738553   -1.4557962625   -2.1897443252
H  3.1758156495   -2.8518325642   -1.1171034774
H  4.6188591415   -0.7329191868   -0.3339927955
H  3.3482140793   -1.181178264    0.7685515338
H  3.1190310549   0.959715732    -1.4181932258
H  3.5280278614   1.2918800262    0.2417503764
H  1.1278021741   1.8111988284   -0.1712363824
Core RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
39.1275           72.0126           104.8047
119.5538          138.7228           175.4244
195.9163          239.6653           349.9199
382.5173          404.8269           465.3001
492.3610          509.7713           668.5910
707.1666          778.0388           783.7805
825.4918          836.9506           898.2100
911.2449          915.0395           945.4280
971.7738          975.4333           985.5970
1011.0730         1038.5237          1055.8517
1100.6413         1113.9880          1117.8712
1132.6002         1158.5182          1181.8776
1208.6659         1260.5213          1288.8473
1294.0628         1309.2533          1328.4999
1347.4890         1360.7243          1370.0232
1381.5000         1390.9768          1459.1689
1468.1926         1481.4261          1486.5148
1494.1870         1679.4634          1729.2589
2925.7019         2980.4892          2988.2796
2998.1709         2999.9316          3000.9874
3014.3776         3047.8071          3053.2517
3120.7384         3127.3798          3133.3165
3165.9709         3190.7129          3234.6574
ZeroEnergy[kcal/mol] 29.64
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----c10h15_R1-3-----
Well      R1-3
Species
RRHO
Geometry[angstrom]  25
C  -1.6177843953   0.5690337396   1.4027875196
C  -1.790869427   -0.8963315313   1.1035201988
C  -1.1274055785  -1.3068072946   -0.2268441264
C   0.2876187998  -0.6892818755   -0.3580870258
C   0.2940189249   0.8540580908   -0.20983818
C  -0.7018209621   1.3378354375    0.814355672

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C  -1.9798813617   -0.9598138091   -1.4039001957
C  1.3297879955   -1.2115946396    0.6777565875
C  1.7483285346    1.154842875    0.2179379085
C  2.0820224982    0.0325360872    1.2161622736
H  -2.2821557392    1.0038951956    2.1454303272
H  -2.8571263057   -1.147869459    1.0718877016
H  -1.3808119618   -1.4890907672    1.9317438915
H  -0.9932748321   -2.4030209603   -0.212214034
H  0.6556135001   -0.9269889599   -1.3617849387
H  0.0710031996    1.3400098847   -1.1673573224
H  -0.6435416695    2.3920064779    1.0787625847
H  -1.5812378767   -1.0381200143   -2.4093889091
H  -3.028001297   -0.7104948011   -1.292253334
H  2.01742201   -1.9109866257    0.1949904574
H  0.849524052   -1.7617982609    1.4906190132
H  1.8699582835    2.1566366624    0.639379057
H  2.4023056798    1.0876924369   -0.6588227752
H  3.1572508863   -0.1348099235    1.3136085636
H  1.7059810421    0.2979790342    2.2076980849
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
42.9511           60.0377           139.3123
167.6286          224.7631           299.1287
327.0699          418.9234           444.3365
477.5439          483.9434           577.1451
607.2819          673.2687           704.2583
777.2706          811.8763           837.0651
849.6476          901.4003           906.0642
922.8648          946.5498           963.4641
977.6006          1005.4061          1012.4687
1032.4867          1055.6635          1087.7303
1101.5204          1138.3983          1153.3149
1186.7561          1192.5512          1213.7608
1251.2289          1266.4451          1277.7646
1291.5488          1314.4966          1319.9166
1346.0503          1349.6508          1356.9925
1372.5878          1378.8154          1424.2137
1456.0762          1483.4555          1491.1654
1496.2619          1513.9438          1713.0901
2909.9022          3001.0637          3006.8492
3018.8542          3027.9698          3030.4875
3038.8175          3047.0556          3066.3972
3070.1905          3090.3704          3116.2185
3128.5195          3143.1051          3230.9260
ZeroEnergy[kcal/mol] 9.56
ElectronicLevels[1/cm] 1
0 2
End
End
!-----

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!-----c10h15_R1-3_i1-----
Well          R1-3_i1
Species
RRHO
Geometry[angstrom]  25
C  -1.598307625    0.6195909429    1.1260611129
C  -1.7189257319   -0.8664834652    1.3210307553
C  -2.8528737507   -1.5206614557    0.5659352262
C   0.9427599618   -0.5495739289   -0.3206063161
C   0.6889809396    0.9132859638   -0.0967211308
C  -0.6223915388    1.3292143462    0.5538931628
C  -3.5729821262   -0.9687229002   -0.4063108579
C   2.0860141649   -1.0593322232    0.5014307129
C   1.9210716154    1.3471344041    0.7619682039
C   2.326171753    0.0730749508    1.523580857
H  -2.4434710386    1.1866910062    1.5136793678
H  -1.867356841    -1.0674283352    2.391748191
H  -0.7836067284   -1.3692842676    1.0538338347
H  -3.0675332403   -2.5460732978    0.862331244
H   0.4287068317   -1.1328602255   -1.0747115029
H   0.7119546279    1.4506905414   -1.0574257357
H  -0.7584185764    2.4106570868    0.5430667574
H  -4.3643418844   -1.5199067429   -0.9017060354
H  -3.3945697211    0.0471636409   -0.7421409546
H   2.9843313081   -1.2131224236   -0.1201619874
H   1.8851609195   -2.0284027594    0.9748910256
H   1.6992673246    2.1885359236    1.4220484843
H   2.7342746431    1.6536461278    0.0957657895
H   3.3540925794    0.1088130165    1.8917564307
H   1.6701561339   -0.066932926    2.3885373649
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
30.0153           34.8327           77.9742
131.2435          145.0111          219.4421
246.6551          295.5860          344.7688
441.8936          453.1941          534.7958
573.7143          598.2289          656.5959
739.1643          768.7291          783.5576
853.2379          876.2308          897.3843
901.9275          928.2351          939.4504
947.0730          967.7362          1018.7475
1026.3534         1031.2472          1037.1517
1039.6510         1073.3958          1104.0508
1142.4623         1187.4913          1215.1288
1236.0583         1255.2907          1288.2079
1304.1998         1314.6996          1325.6532
1333.1035         1341.4606          1347.3752
1366.2451         1428.3052          1445.3728
1464.8629         1471.7576          1490.4436
1504.1337         1702.3531          1714.6460

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2932.5791          2952.4366          2988.2612
3009.6425          3029.9368          3036.7753
3037.6990          3079.1508          3087.4518
3095.7166          3118.6106          3123.2043
3135.2154          3187.6036          3214.4208
ZeroEnergy[kcal/mol] 30.11
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----c10h15_R1-3_i2-----
Well      R1-3_i2
Species
RRHO
Geometry[angstrom]  25
C  -0.89942156    0.4353089047    0.583350219
C  -0.6780599225   -1.0270746992    0.3253438351
C  -1.8878191444   -1.7719930808    -0.1911230608
C   2.1949372627    0.7555781991   -0.4473594015
C   1.0515082597    1.4067693806   -0.6993102084
C  -0.1634947812    1.4582809051    0.1298971453
C  -3.0042908713   -1.2329745374   -0.6715089523
C   2.5350140349   -0.0467615673    0.7766385857
C   5.0683756703   -0.0675996578    0.4814892806
C   3.9238319784    0.3119375214    1.3553544522
H  -1.7778539265    0.6721061364    1.1797888762
H  -0.3524292987   -1.5169815552    1.2551310115
H   0.1486895816   -1.1653276495   -0.3799075221
H  -1.7976114416   -2.8565629042   -0.168974905
H   2.9980274493    0.8492319282   -1.1759514938
H   1.0174647827    2.0240592719   -1.5963652208
H  -0.5209297667    2.4631981897    0.3530415101
H  -3.8163456668   -1.8537127098   -1.0327863672
H  -3.1455881038   -0.1591522998   -0.7306572358
H   2.5348488396   -1.1188877962    0.5335919286
H   1.7703753552    0.0980848876    1.5437377109
H   5.9928735223    0.4960996626    0.4873250456
H   5.0540946667   -1.0051712503   -0.0639967139
H   4.0167204487   -0.1985124229    2.3299736857
H   3.9597236315    1.3830971429    1.5835887952
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
41.2492          43.2095          76.5771
105.9283         129.9542         134.8736
153.4325         168.5193         247.6607
263.1053         371.6151         388.1551
470.6932         511.0348         527.6606
544.4637         605.3616         689.5845
772.2511         787.2838         808.9798

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871.6483	888.6894	909.2731
940.9380	942.1396	956.9734
1007.2137	1016.0497	1033.3601
1046.3835	1053.1056	1083.5454
1107.1873	1111.0733	1194.8066
1223.5032	1243.2268	1274.8235
1288.7805	1328.8188	1338.6968
1348.6214	1360.9170	1419.8959
1444.1083	1454.8736	1461.0729
1466.0378	1468.8966	1485.4696
1694.2712	1698.2654	1706.0926
2923.0495	2981.2034	2988.0060
3035.1100	3043.2519	3074.0330
3099.6818	3107.9757	3121.3199
3129.6169	3132.7077	3135.1860
3138.3929	3214.5477	3232.1107
ZeroEnergy[kcal/mol] 42.54		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----c10h15_R1-3_i3-----		
Well R1-3_i3		
Species		
RRHO		
Geometry[angstrom] 25		
C	-1.5577387872	0.9110722774 -0.2384449062
C	-1.7742843406	-0.1471513864 0.8088587173
C	-2.604343757	-1.3293763968 0.3599078796
C	1.1866175927	-0.6109120732 -0.9385005752
C	1.0099819228	0.846001416 -0.5777317552
C	-0.4207127451	1.3213908594 -0.806405775
C	-2.9293081135	-1.6313665991 -0.8935445979
C	1.9968945687	-1.0614092411 -1.8923876905
C	1.5172577376	1.1667235187 0.8610092829
C	2.9803072179	0.9678055454 1.0440998583
H	-2.4739718373	1.3956023075 -0.571125866
H	-2.2835620639	0.3126044603 1.6679288676
H	-0.8256307189	-0.5192973029 1.2082874391
H	-2.9425625888	-1.9808429648 1.1637610975
H	0.5923548514	-1.3248087401 -0.3728284951
H	1.6449465953	1.4214530564 -1.2589548454
H	-0.5110022227	2.1099747043 -1.5498111408
H	-3.5235064248	-2.5087725526 -1.1225063936
H	-2.6095681783	-1.0207111038 -1.7309761918
H	2.6024948607	-0.3866977366 -2.4903003749
H	2.079419337	-2.1194749369 -2.1149854784
H	0.954938209	0.5471530884 1.5786047996
H	1.2425495251	2.199599918 1.1043208084
H	3.5219435357	1.5240572341 1.7991525499
H	3.5024098242	0.1791486483 0.5166267856

```

Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
30.9507          57.9703          90.2382
95.7878          130.3898         139.7354
151.9422         181.5852         250.2911
273.5061         301.6621         387.1999
441.3630         445.4457         495.9288
551.3685         604.5352         656.4138
715.9366         742.7185         757.3096
879.3721         903.5446         942.0986
943.4293         949.9090         965.8622
994.6829         1014.9168        1025.4300
1035.1450        1046.6768        1060.7399
1092.4701        1106.3702        1148.3190
1194.1735        1242.3493        1303.5724
1320.7307        1327.2067        1329.5110
1336.5837        1342.1301        1362.1451
1426.6675        1447.2917        1452.0670
1456.9474        1463.8184        1475.9826
1696.6535        1704.0598        1713.3411
2944.4957        2991.1513        3026.1629
3034.7533        3049.6391        3114.0490
3121.1043        3122.1864        3137.4839
3138.5375        3139.2760        3140.0601
3206.9815        3216.8953        3241.9352
ZeroEnergy[kcal/mol] 47.80
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R1-3_i4-----
Well          R1-3_i4
Species
RRHO
Geometry[angstrom] 25
C -1.8687999115 2.0683062058 0.5381189677
C -2.5104244613 2.4165221402 -0.6343556534
C -0.6584320283 1.3940284221 0.6695926218
H -2.3619403945 2.3481636059 1.4671203862
H -3.4536139601 2.9474005165 -0.6117034368
H -2.1095821082 2.1678538189 -1.6089521666
H -0.3169519281 1.1841080043 1.679871272
C -1.1887739738 -1.2022898436 -0.837248333
C 0.1787880617 -0.6020628599 -0.7255846592
C 0.2308917009 0.942675407 -0.4500895217
C -1.6450824714 -1.8736029734 -1.8916713357
C 1.0471795679 -1.1972396679 0.4117409037
C 1.7270810069 1.1296041445 -0.0963619827
C 2.11402768 -0.1170289561 0.7401553224

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H  -1.836245792   -1.0701457831   0.027611925
H  0.7036331778   -0.7594420615   -1.6758624891
H  -0.0273234184   1.4830665789   -1.3637415027
H  -1.0345035534   -2.0268514433   -2.7770296133
H  -2.6442044522   -2.2944533325   -1.9101729966
H  1.4861490059   -2.1509665078   0.1113094323
H  0.4220611493   -1.4019711554   1.2860596386
H  1.916579007    2.0688916216   0.4280741182
H  2.3074159396    1.1557052616   -1.0237245175
H  3.1238151631   -0.4548608804   0.4963655008
H  2.114601993    0.1120407376   1.8087351196
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
35.0469           77.1235           84.4575
105.6628          174.3690          217.8612
251.3082          282.4658          370.1863
382.5611          468.4026          540.5882
559.5646          619.4901          655.9355
687.9264          753.3582          788.8801
791.4409          842.0758          869.4065
890.5572          941.0126          954.4337
972.6879          992.3570         1002.9795
1010.2015         1029.1063         1034.7190
1046.1386         1083.9630         1135.6789
1169.1279         1207.7915         1217.9569
1228.6009         1240.5219         1280.2054
1285.1552         1297.4783         1320.8467
1326.1454         1328.4560         1348.0541
1359.2756         1440.4611         1459.7741
1483.1437         1493.4915         1498.8963
1518.5104         1528.6475         1702.7124
3007.9591         3033.4342         3035.9531
3049.2824         3065.8601         3067.2797
3081.8824         3093.9376         3119.9590
3120.9174         3130.0923         3144.4814
3151.5235         3205.9815         3238.4547
ZeroEnergy[kcal/mol]  16.49
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----c10h15_R1-3_i5-----
Well          R1-3_i5
Species
RRHO
Geometry[angstrom]  25
C  -1.9600232621   0.5781877497   0.877688772
C  -2.4642808976  -0.619825149   0.117830481
C  -1.6922327343  -0.9181370064  -1.1307797244

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C	-0.2782063274	-0.442457012	-1.2259193572
C	-0.0660240329	1.0089300936	-0.7158893407
C	-0.9065444979	1.3016204592	0.5022811987
C	-2.1921280441	-1.98846644	-2.0446942974
C	0.7577827352	-1.3006237376	-0.3996954822
C	1.4446540508	1.0578062304	-0.4108299456
C	1.7384568756	-0.2968679829	0.2596748982
H	-2.5121625483	0.8554823626	1.772019245
H	-3.5274840333	-0.4741773709	-0.1273695867
H	-2.4686391391	-1.4968472491	0.7952172122
H	0.0325851542	-0.4767168127	-2.2765193971
H	-0.3207333642	1.7322402309	-1.5005434199
H	-0.6178098171	2.1680172892	1.0942396977
H	-1.9475865136	-3.0003317479	-1.6759000834
H	-1.7522987972	-1.9047280696	-3.0435584663
H	-3.2824902853	-1.955426351	-2.1489871996
H	1.2740031719	-1.9988854358	-1.0627820085
H	0.2475251563	-1.9020365741	0.3561499853
H	1.7255025574	1.9127034094	0.2108680924
H	1.9988700713	1.1439665899	-1.3519951142
H	2.7831694293	-0.5967400314	0.147341205
H	1.5378620926	-0.2289674447	1.3320416357

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 69

41.4273	76.8429	116.5601
145.5925	163.6347	269.9874
325.2628	412.4977	431.3224
451.8630	484.4908	604.0284
624.2175	682.3851	783.1682
799.6773	837.8014	840.1525
891.6845	900.5909	916.1824
931.0534	955.9021	990.9138
1004.5443	1007.0841	1014.9751
1023.0481	1050.0763	1093.6028
1151.8105	1176.3896	1187.1909
1195.1661	1196.9725	1247.9963
1268.5015	1293.4931	1303.0544
1305.9046	1331.0990	1333.0133
1343.5216	1359.1536	1401.7482
1405.2426	1420.6396	1455.6040
1475.5307	1487.0681	1488.2380
1496.7999	1512.7413	1714.5479
2879.3822	2924.7165	2971.0511
3000.5927	3011.4985	3022.8806
3027.2969	3039.0418	3049.5980
3064.9659	3069.4022	3072.6899
3093.0513	3118.2172	3145.9813

ZeroEnergy[kcal/mol] 4.30

ElectronicLevels[1/cm] 1

0 2

```

End
End
!-----
!-----c10h15_R1-3_i6-----
Well          R1-3_i6
Species
RRHO
Geometry[angstrom]  25
C  -0.7432720081    2.6734645954    3.2967353327
C  -1.9551344118    2.1375084685    3.1269144113
C   0.5210012004    2.1351395022    2.7806997433
C  -1.0271266631    -2.0878938909    -0.0139276594
C  -0.0804578013    -1.1281003568    -0.3440969593
C   0.6737586287    1.452882184    1.6392754274
C  -2.3942292067    -1.9447513816    -0.1496245342
C   1.39676253    -1.309433585    -0.1749142951
C   1.9786811543    0.8821679314    1.1596570804
C   2.0299107561    -0.662463289    1.0835417921
H  -0.658792093    3.5835746595    3.8880787466
H  -2.8421058054    2.6149823607    3.5267897472
H  -2.0971860684    1.2016601951    2.5966652235
H   1.4049628235    2.3419960303    3.383238196
H  -0.6569146135    -3.032958122    0.3827759494
H  -0.4335439651    -0.1850593343    -0.7545866479
H  -0.1976913833    1.2958617428    1.0095303844
H  -2.8267941989    -1.0304654199    -0.541340385
H  -3.0754286065    -2.7393981613    0.1259112193
H   1.9156011584    -0.9092453048    -1.0560331064
H   1.621832366    -2.3814106599    -0.1418424463
H   2.7725331362    1.2206467766    1.8333258612
H   2.2211585028    1.2879814369    0.167604279
H   3.0828578068    -0.9655341984    1.1018719727
H   1.5671547619    -1.0836761795    1.981831667
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
22.7336           31.5905           68.7598
85.1716           130.9616          156.7320
184.5684          236.8051          265.0841
303.8259          349.1587          377.2468
465.3390          507.8045          553.7285
595.2876          654.0447          759.5679
795.2116          800.3775          840.0592
857.9613          878.4118          938.4275
947.3998          972.5881          997.8450
999.3727          1024.2261         1033.7893
1039.6009          1057.8595         1097.6536
1138.9161          1176.3840         1206.6425
1239.1695          1261.8464         1289.3478
1314.4528          1325.7664         1346.6789
1349.8944          1357.5340         1374.8987

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1385.1837	1452.5500	1481.3912
1485.7128	1487.9327	1497.5358
1519.4193	1677.2863	1705.1286
2991.0035	2995.5571	3015.1838
3041.0503	3049.9010	3061.9315
3107.5652	3111.2339	3124.0366
3133.6276	3135.6797	3138.7538
3151.5924	3217.8106	3232.7924

ZeroEnergy[kcal/mol] 30.59

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h15_R1-3_i7-----

Well R1-3_i7

Species

RRHO

Geometry[angstrom] 25

C	-1.7851635469	1.2225676638	0.991375685
C	-2.1467707075	-0.1652880664	0.524807098
C	-1.2976839114	-0.6294462952	-0.6914547475
C	0.1336277973	-0.256640106	-0.4657076136
C	0.471858368	1.159110709	-0.0805640837
C	-0.6268911499	1.8221021321	0.7116273545
C	-1.5295941687	-2.1104281059	-1.0084907118
C	1.3108004045	-1.1682020094	-0.2706399085
C	1.8267134093	1.0155271295	0.663542062
C	2.486485648	-0.1988268736	-0.0128043164
H	-2.5258459395	1.748611621	1.5886254029
H	-3.211589065	-0.204067806	0.2630810983
H	-2.0163861112	-0.8790409321	1.3510355734
H	-1.6653054829	-0.0397038384	-1.5483628484
H	0.6498911167	1.7713250285	-0.9856456346
H	-0.4417256659	2.8336062368	1.0661185654
H	-1.1957777307	-2.7508596921	-0.1864169705
H	-0.990840108	-2.414381756	-1.9097964966
H	-2.5925609264	-2.3091848736	-1.1729830114
H	1.4950000279	-1.8367282219	-1.120893764
H	1.1664471367	-1.8305897547	0.6000741818
H	1.6339388476	0.7974694006	1.7196651412
H	2.4380435952	1.9205311678	0.617746085
H	2.9287903359	0.1046417776	-0.9676723716
H	3.282226827	-0.6428015354	0.5899642311

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 69

62.1450	99.1130	176.4960
212.5065	241.9793	256.4508
312.4584	419.6346	427.0077
452.0635	523.4319	550.3793

576.6703	673.0989	724.5970
771.5015	850.6508	873.3110
884.4208	908.7673	919.2838
929.9045	981.3900	998.4017
1000.1019	1013.9229	1036.4032
1051.4259	1092.1185	1096.5161
1122.3669	1168.4044	1183.8264
1200.1478	1223.0383	1231.3837
1260.5604	1292.6687	1293.7991
1315.5290	1321.7706	1330.5335
1343.4004	1348.6468	1387.6103
1409.3591	1413.8615	1472.7311
1479.5227	1492.5261	1500.8869
1502.5740	1506.5527	1704.5140
2881.3149	2924.8368	2927.7185
2984.3823	3004.3613	3019.2331
3023.2598	3025.5247	3031.4086
3073.9980	3082.6997	3083.0208
3089.6237	3121.9374	3146.2367

ZeroEnergy[kcal/mol] 4.06

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c2h3_c8h12_R1-1_p1-----

Bimolecular R1-1_p1

Fragment c8h12

RRHO

Geometry[angstrom] 20

C	-0.0045524871	1.6804549839	-0.2310000936
C	-1.192873494	1.1058911041	-0.0475446203
C	1.5004724486	-1.0803032458	0.7302571069
C	1.9211709929	0.1173985555	0.324781107
C	1.2824201067	1.0303326169	-0.7066793302
C	-1.6568321854	-0.3110177755	-0.2761249313
C	0.3241881253	-1.9190405595	0.2966321836
C	-0.6753670812	-1.3967647594	-0.7493571781
H	0.0722096814	2.7369487533	0.0135911155
H	-1.9888927052	1.7524925863	0.3194548848
H	2.0992057348	-1.5659673255	1.4997289828
H	2.8135639908	0.5118157016	0.8043219741
H	1.9950994965	1.8208187657	-0.9528585338
H	1.1124570664	0.4891849527	-1.639344002
H	-2.4794532241	-0.261682942	-1.0036391942
H	-2.1345297384	-0.6586417975	0.6512120278
H	-0.2367293334	-2.198317436	1.200176457
H	0.7325883097	-2.8697832947	-0.0744535194
H	-0.1589430136	-1.0843507227	-1.6586822288
H	-1.2866376907	-2.2559571614	-1.0475342077

Core RigidRotor

SymmetryFactor 1

```

End
Frequencies[1/cm]  54
8.9281              197.9085              266.4791
276.5764            311.1976              388.2911
400.0393            528.4433              638.1972
667.2851            715.5347              721.3852
788.5349            833.9261              878.3359
880.0639            925.3593              1004.2965
1005.1795           1006.9931              1016.9616
1035.3217           1095.0834              1115.5955
1177.1316           1220.6754              1259.5375
1283.8701           1299.6732              1306.1121
1339.8245           1381.4809              1400.5446
1402.7706           1423.1453              1432.4164
1463.7679           1475.5395              1489.1124
1521.5391           1721.1316              1730.7871
2981.9789           2982.5760              2996.8343
2997.9189           3028.9273              3052.2833
3073.4239           3095.5935              3105.9317
3107.9005           3137.4621              3142.1446
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment            c2h3
RRHO
Geometry[angstrom]  5
C  -2.6815309499    -1.8887734891    -1.1309235268
C  -1.725733176     -1.3518528792    -0.4241833636
H  -3.0692157655    -1.4200651964    -2.0332260024
H  -3.1437000229    -2.8401606701    -0.8523521394
H  -1.1628990858    -1.5707617651     0.4715150322
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  9
712.2118            819.4319              921.7170
1046.2369           1391.3607              1651.0507
3037.2336           3133.0072              3234.0563
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol]  66.20
End
!-----c4h6_c6h9_R1-1_p2-----
Bimolecular  R1-1_p2
Fragment      c6h9
RRHO
Geometry[angstrom]  15
C  0.8437509359     0.9604783141     0.7729854028
C  1.5670660402     1.9073686626     1.3819587486

```

```

C  -0.20495359    0.0748761654   -1.3257446705
C  0.5269521747    0.9734296574   -0.6476094819
C  -0.8695548974   -1.1679090018   -0.7900192351
C  -0.3229094284   -2.4216099648   -1.395655044
H  0.4711275423    0.1303724266    1.3664916365
H  1.7848370785    1.8633602508    2.4422803345
H  1.9636943703    2.7569847806    0.8346501872
H  -0.3339448586    0.2312064941   -2.3939900439
H  0.936559286    1.813057982   -1.2055542041
H  -1.9473967655   -1.1097730338   -0.9901563709
H  -0.7801971782   -1.2064850793    0.3057852915
H  -0.9597388586   -3.2776234404   -1.5811260648
H  0.7424711487   -2.5278922135   -1.559294486
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  39
47.3969            108.6574            130.4201
213.1922           258.7611            380.7756
436.9677           495.3619            607.4627
676.1322           793.6205            820.2181
908.8488           931.5385            987.4361
994.9143           1038.4625           1047.4122
1086.8052          1151.5663           1224.4669
1290.1770          1319.4203           1331.1399
1399.3067          1455.5816           1462.0681
1471.3704          1652.7846           1704.0838
2969.5175          3011.9325           3120.2458
3130.8462          3135.8492           3144.7430
3150.2230          3218.9507           3242.7186
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
Fragment          c4h6
RRHO
Geometry[angstrom]  10
C  0.0  -1.843324    0.133025
C  0.0  -0.613696   -0.391646
C  0.0   0.613696    0.391646
C  0.0   1.843324   -0.133025
H  0.0  -2.728775   -0.491109
H  0.0  -2.000484    1.20716
H  0.0  -0.495039   -1.473421
H  0.0   0.495039    1.473421
H  0.0   2.000484   -1.20716
H  0.0   2.728775    0.491109
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  24
174.2767           297.9228           518.5211

```

```

538.7597          780.9904          899.0718
935.4151          936.3573        1000.6886
1003.8829         1057.4243        1226.5960
1314.7435         1319.7664        1415.4322
1473.2852         1652.9463        1705.8417
3121.7476         3130.9783        3134.5251
3135.1337         3218.8231        3219.2522
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
GroundEnergy[kcal/mol] 62.38
End
!-----c2h4_c8h11_R1-1_p3-----
Bimolecular      R1-1_p3
Fragment          c8h11
RRHO
Geometry[angstrom]      19
C  2.0069210336   1.2462451866   0.1465129964
C  2.0780616429   2.0666980102   1.1907424041
C  -0.8512401985   1.3044782128   -0.9946375095
C  -2.1541631237   1.1944692997   -0.9738532863
C  1.9632483622   -1.2103421392   -0.0105660516
C  1.1023390037   0.0369909243   0.0400443918
C  0.1223881389   0.1596614752   -1.1496104471
C  2.0591485532   -2.0859652981   -1.0071986596
H  2.651014671    1.4177030556   -0.7152057052
H  2.7605832265    2.9091912379   1.2060282145
H  1.4558437496    1.9248188537   2.0692884006
H  -0.4034457849    2.2988107091   -0.8827241478
H  -3.012767832    1.8430781826   -0.8822045912
H  2.573119216     -1.3599725291   0.8782735015
H  0.5065438745     -0.0143669569   0.9606664191
H  0.6978922599     0.3031392259   -2.0730583657
H  -0.4353535216     -0.7730066882   -1.2584237506
H  2.723045289      -2.9401354327   -0.9355561749
H  1.4871674395     -1.9960083293   -1.9235906385
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  51
74.5213           87.5766           100.2543
102.4510          192.9812           272.4975
312.7586          347.9478           385.1290
443.7223          564.4640           623.9156
668.0200          695.8510           786.0590
827.3156          853.9582           942.8407
948.8619          951.4391           966.5376
1000.2228         1034.3992          1039.8431
1062.4768         1131.4820          1143.0404
1225.9506         1261.5105          1291.6314
1318.4832         1320.9639          1338.0803

```

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1360.5901          1447.6829          1451.7247
1486.4048          1676.4411          1691.5359
1703.6850          3001.5980          3014.2561
3022.9136          3082.8243          3115.7897
3125.1966          3127.9860          3141.3649
3208.9669          3216.8698          3236.4230
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  2
End
Fragment      c2h4
RRHO
Geometry[angstrom]      6
C  0.0    0.6634900906    0.0
C  0.0   -0.6634900906    0.0
H  0.0    1.23462754   -0.9225248038
H  0.0    1.23462754    0.9225248038
H  0.0   -1.23462754    0.9225248038
H  0.0   -1.23462754   -0.9225248038
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm]  12
834.2929          972.9227          974.1218
1066.8559         1238.5875         1379.4650
1472.0483         1691.5384         3121.2072
3136.3255         3192.3844         3220.8390
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
GroundEnergy[kcal/mol]  77.92
End
!-----c5h7_c5h8_R1-2_p6-----
Bimolecular      R1-2_p6
Fragment      c5h8
RRHO
Geometry[angstrom]      13
C  -0.665756    1.185494   -0.054519
C   0.665753    1.185496   -0.054519
C  -1.234872   -0.207474    0.092831
C   1.234873   -0.20747    0.092831
C   2.0E-6   -1.117143   -0.141641
H  -1.288049    2.071583   -0.111515
H   1.288042    2.071588   -0.111515
H  -1.657658   -0.343488    1.097383
H  -2.04568    -0.414198   -0.612849
H   2.045682   -0.414191   -0.612849
H   1.657659   -0.343482    1.097383
H   3.0E-6   -1.464314   -1.178358
H   4.0E-6   -2.002396    0.497331
Core RigidRotor

```

```

SymmetryFactor 1
End
Frequencies[1/cm]  33
145.0227          394.0659          615.2119
715.0038          783.2473          820.6523
890.9966          902.7539          916.9280
972.5321          973.7944        1035.1036
1068.3393         1129.2698         1154.1645
1223.8342         1231.5469         1308.6237
1319.1067         1326.6826         1377.9063
1484.9848         1490.4453         1509.6503
1679.7423         2995.1374         2996.6206
3034.5877         3043.4115         3054.4307
3089.8961         3165.1862         3190.1907
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment          c5h7
RRHO
Geometry[angstrom]  12
C  -1.236049    -0.322875    -4.7E-5
C  -0.666035     1.080029    -1.54E-4
C   0.666039     1.080025    -9.3E-5
C   1.236047    -0.322881     1.6E-5
C  -2.0E-6     -1.172611    -7.8E-5
H  -1.882518    -0.504585    -0.874435
H  -1.882364    -0.504494     0.874482
H  -1.291027     1.9654     -2.5E-4
H   1.291038     1.965392    -1.37E-4
H   1.882314    -0.504505     0.874579
H   1.882565    -0.504584    -0.874337
H  -8.0E-6     -2.254306     4.58E-4
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  30
206.3392          331.6291          390.6560
682.3568          742.2851          791.8872
896.2936          912.6840          923.9412
944.1444          960.9987          969.9333
1033.7395         1127.4785         1128.9131
1131.2069         1273.6783         1299.0661
1323.7078         1386.4351         1456.9616
1462.8643         1675.8106         2943.2234
2943.7650         2944.1189         2948.0656
3171.9185         3196.2535         3203.9518
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol]  32.27

```

```

End
!-----c2h4_c8h11_R1-2_p1-----
Bimolecular    R1-2_p1
Fragment       c8h11
RRHO
Geometry[angstrom]  19
C  -2.7342652128    0.0868348208    0.1142223458
C  -2.17523837     0.8708570487    1.0339971935
C  -0.6657869164    0.7997156964    0.9967141277
C  -0.3998700166    -0.4732347302    0.1496030959
C  -1.6992090855    -0.6539149341    -0.6980813907
C  0.865589892     -0.5320380491    -0.6470782032
C  3.1171985769     0.2134977531    -1.2841406194
C  1.9523577186     0.3223051836    -0.5460238216
H  -3.7988001954    0.0092568819    -0.0759145497
H  -2.7157165273    1.5281096467    1.7057056102
H  -0.2084556906    0.7429052029    1.9891852271
H  -0.2611562631    1.6992271408    0.5138423326
H  -0.3915406177    -1.3192541392    0.8544631028
H  -1.5903897173    -0.1995306465    -1.6920421579
H  -1.9424543037    -1.7089934153    -0.8582067352
H  0.9422161521     -1.3611600609    -1.3493308294
H  3.2481342117     -0.5783721538    -2.013667951
H  3.9323757046     0.9142474078    -1.1580698877
H  1.8908876604     1.1410603461    0.1673451102
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  51
63.8015            104.0616            158.9477
189.0436           357.5374            379.2804
404.2592           496.1074            547.1269
657.7944           705.9635            759.0884
778.8509           795.9983            831.2846
914.8626           943.9012            962.5313
972.7504           976.0345            994.9048
1027.8009          1046.1388           1124.2622
1132.4915          1156.3160           1199.5800
1213.1770          1281.8005           1286.6122
1293.8460          1307.6878           1339.3387
1356.6498          1374.4126           1487.9488
1494.9522          1499.4856           1522.2185
1679.8045          2953.3989           2998.6192
3000.0307          3049.4063           3053.4186
3115.2666          3135.9380           3138.1764
3167.5727          3192.0912           3232.8217
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
Fragment          c2h4
RRHO

```

```

Geometry[angstrom] 6
C 0.0 0.6634900906 0.0
C 0.0 -0.6634900906 0.0
H 0.0 1.23462754 -0.9225248038
H 0.0 1.23462754 0.9225248038
H 0.0 -1.23462754 0.9225248038
H 0.0 -1.23462754 -0.9225248038
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm] 12
834.2929 972.9227 974.1218
1066.8559 1238.5875 1379.4650
1472.0483 1691.5384 3121.2072
3136.3255 3192.3844 3220.8390
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 37.28
End
!-----c2h4_c8h11_R1-3_p1-----
Bimolecular R1-3_p1
Fragment c8h11
RRHO
Geometry[angstrom] 19
C -1.1216782175 1.207395685 0.3418688752
C -1.1905602702 -0.004527097 1.2253405494
C -1.9682619161 -1.1855719247 0.681772053
C 1.4220159824 -0.4498693704 -0.7316613954
C 1.060641928 0.9081455219 -0.9193490063
C -0.1269274996 1.5749000319 -0.5243878491
C -2.4637620891 -1.3050413534 -0.5459998968
C 2.6167835381 -0.973581268 -1.1197069254
H -1.9588246814 1.894023907 0.4329476281
H -1.6591327648 0.2878651703 2.17475424
H -0.1830829558 -0.3422824688 1.4962208748
H -2.1144054632 -1.9967872256 1.3931527443
H 0.6932130089 -1.1214839801 -0.2910911613
H 1.773406346 1.511534846 -1.4771272592
H -0.2513200228 2.5585094428 -0.9732301239
H -3.0079155001 -2.1930473121 -0.8469280728
H -2.3404962832 -0.5247585109 -1.2893396748
H 3.3804101735 -0.3566976602 -1.582310907
H 2.846024687 -2.0228684338 -0.9821556928
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 51
51.5769 91.6207 109.1156
147.3840 218.9561 242.4711
303.4287 412.9394 453.0338

```

554.5531	581.9664	613.2688
717.9676	744.1054	827.5742
857.7396	870.1531	906.9965
946.2102	955.2154	970.5210
1009.9468	1024.0329	1038.9205
1078.9415	1114.3450	1200.8051
1233.7700	1267.2936	1314.0500
1321.1764	1343.8896	1375.5166
1437.9416	1456.9702	1464.5255
1484.9847	1536.0018	1586.7785
1702.4799	2997.5563	3026.8848
3114.3297	3118.8313	3131.9512
3135.7568	3136.2745	3149.5838
3172.4795	3216.7689	3227.3421
ZeroEnergy[kcal/mol]		0.0
ElectronicLevels[1/cm]		1
0 2		
End		
Fragment		c2h4
RRHO		
Geometry[angstrom]		6
C	0.0	0.6634900906 0.0
C	0.0	-0.6634900906 0.0
H	0.0	1.23462754 -0.9225248038
H	0.0	1.23462754 0.9225248038
H	0.0	-1.23462754 0.9225248038
H	0.0	-1.23462754 -0.9225248038
Core RigidRotor		
SymmetryFactor		4
End		
Frequencies[1/cm]		12
834.2929	972.9227	974.1218
1066.8559	1238.5875	1379.4650
1472.0483	1691.5384	3121.2072
3136.3255	3192.3844	3220.8390
ZeroEnergy[kcal/mol]		0.0
ElectronicLevels[1/cm]		1
0 1		
End		
GroundEnergy[kcal/mol]		47.32
End		
!-----c4h6_c6h9_R1-3_p2-----		
Bimolecular		R1-3_p2
Fragment		c6h9
RRHO		
Geometry[angstrom]		15
C	-0.8957529004	1.4520632614 1.2341143102
C	-2.0813755431	0.8589491659 1.0704519911
C	0.4006434998	0.9401710473 0.7748077354
C	0.6087549197	0.2026408034 -0.3218913908
C	1.9473902001	-0.3428722371 -0.7509296588
C	1.9870976304	-1.8378005448 -0.7571476904

```

H -0.8609693618    2.3961527446    1.7748143592
H -2.995226575    1.3205966743    1.4255563653
H -2.1751619122   -0.1088598732    0.5891701271
H  1.2622437483    1.2201820436    1.3798713694
H -0.2328402795   -0.0431258877   -0.9661439179
H  2.7228238917    0.0574718902   -0.0773027371
H  2.194911012    0.0315226665   -1.7520226393
H  2.4878275673   -2.3864625524   -1.5448864333
H  1.5818331026   -2.3936752021    0.0796752098
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  39
75.1985           93.7542           113.3620
186.2553          241.6258           354.6496
396.6414          495.8077           598.3363
651.9936          786.7289           865.8898
935.1045          960.5744           998.6706
1018.4684         1029.9946          1047.8607
1084.3161         1114.2923          1208.6631
1308.5759         1320.4064          1343.1995
1350.5157         1451.5475          1458.2124
1461.9844         1676.3280          1703.4821
2944.5921         3019.5522          3109.5336
3125.8006         3133.5765          3136.0619
3137.7458         3218.0992          3243.4925
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
Fragment          c4h6
RRHO
Geometry[angstrom]  10
C  0.0  -1.843324    0.133025
C  0.0  -0.613696   -0.391646
C  0.0   0.613696    0.391646
C  0.0   1.843324   -0.133025
H  0.0  -2.728775   -0.491109
H  0.0  -2.000484    1.20716
H  0.0  -0.495039   -1.473421
H  0.0   0.495039    1.473421
H  0.0   2.000484   -1.20716
H  0.0   2.728775    0.491109
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  24
174.2767          297.9228           518.5211
538.7597          780.9904           899.0718
935.4151          936.3573          1000.6886
1003.8829         1057.4243          1226.5960
1314.7435         1319.7664          1415.4322

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1473.2852          1652.9463          1705.8417
3121.7476          3130.9783          3134.5251
3135.1337          3218.8231          3219.2522
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
GroundEnergy[kcal/mol] 60.23
End
!-----ch3_c9h12_R1-3_p4-----
Bimolecular      R1-3_p4
Fragment         c9h12
RRHO
Geometry[angstrom]      21
C  -1.9427907026      0.7964928021      0.859725906
C  -2.1519411467      -0.6514942638      0.4947326768
C  -1.3227515257      -1.0807777782      -0.6893812703
C  -0.714121931       -0.2097821454      -1.4895261777
C  -0.774431522       1.2884994972      -1.2767364416
C  -1.3087074538      1.6665324852      0.0753924552
C   0.265271849       -0.5003498431      -2.6139276855
C   0.6652801752      1.7241816557      -1.6309864423
C   1.0033719455      0.8483138128      -2.8560891052
H  -2.3380623932      1.1218183965      1.8182841119
H  -3.2221165378      -0.8355294166      0.3095335692
H  -1.9097803455      -1.2845910543      1.3592722222
H  -1.2018815031      -2.1496695332      -0.8499762305
H  -1.4356159219      1.7251390188      -2.0455747648
H  -1.1904787403      2.6996561925      0.3925073178
H  -0.2449828198      -0.8414226666      -3.5204158597
H   0.958065743       -1.2955442911      -2.325029724
H   1.3286875877      1.4855500325      -0.7927315129
H   0.7547294066      2.7943888607      -1.8350770731
H   0.6219879516      1.3264938364      -3.7633915415
H   2.0786458848      0.7169304018      -2.9929694301
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  57
60.9326          165.3712          220.5226
284.2798          354.1734          435.5230
499.1243          533.0340          583.9274
627.7226          704.4476          753.0366
795.0536          835.7740          858.6370
888.1116          906.1178          916.6116
972.7027          990.1776          1007.9388
1017.3507         1030.7511          1068.9087
1087.5723         1134.5350          1163.5186
1196.6217         1197.3968          1215.5318
1238.9301         1289.1236          1303.6701
1308.9012         1331.1794          1336.5863
1366.6434         1385.5174          1417.2544

```

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1473.8600          1480.4379          1494.6358
1510.3690          1702.6337          1756.4172
2928.7688          2962.5677          2997.8620
3026.2871          3028.5941          3038.7298
3059.2743          3076.0615          3089.5046
3129.6080          3130.9177          3153.5573
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment      ch3
RRHO
Geometry[angstrom]      4
C  0.0  1.995E-7  0.0
H  0.0  1.0804553795  0.0
H  0.9357017515  -0.5402277895  0.0
H -0.9357017515  -0.5402277895  0.0
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  6
505.1501          1403.0831          1403.0885
3103.6402          3282.6573          3282.6683
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol] 26.29
End
!-----c5h8_c5h7_R1-3_p6-----
Bimolecular      R1-3_p6
Fragment      c5h7
RRHO
Geometry[angstrom]      12
C  0.7002153115  0.2843490193  0.9798752969
C  0.2502074535  -0.9301307528  0.2032432565
C -0.9351407558  -0.7044779376  -0.70505908
C  1.8784644636  0.8457990836  0.906763262
C -1.4609528823  0.4699770661  -1.0379588598
H -0.0475821445  0.7093596836  1.6608150481
H -0.0092026067  -1.7247780934  0.9164070483
H  1.0886908941  -1.3205698489  -0.3843587463
H -1.3706461822  -1.6130009516  -1.1170634174
H  2.4035909977  1.6754620954  1.3560297507
H -2.3121700592  0.5344571341  -1.706027953
H -1.0568404897  1.4053205022  -0.6659956058
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  30
94.8582          149.5878          261.2712
397.3667          512.4018          573.0544

```

670.2951	779.9040	828.2481
907.5879	938.5203	953.1000
1031.0037	1045.8123	1109.2237
1207.1310	1275.5054	1326.0602
1348.6860	1444.8420	1467.7422
1678.3461	1706.4159	2996.6459
3011.7763	3040.5163	3122.1637
3137.3209	3216.2544	3239.3211

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 2

End

Fragment c5h8

RRHO

Geometry[angstrom] 13

C -0.665756 1.185494 -0.054519

C 0.665753 1.185496 -0.054519

C -1.234872 -0.207474 0.092831

C 1.234873 -0.20747 0.092831

C 2.0E-6 -1.117143 -0.141641

H -1.288049 2.071583 -0.111515

H 1.288042 2.071588 -0.111515

H -1.657658 -0.343488 1.097383

H -2.04568 -0.414198 -0.612849

H 2.045682 -0.414191 -0.612849

H 1.657659 -0.343482 1.097383

H 3.0E-6 -1.464314 -1.178358

H 4.0E-6 -2.002396 0.497331

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 33

145.0227	394.0659	615.2119
----------	----------	----------

715.0038	783.2473	820.6523
----------	----------	----------

890.9966	902.7539	916.9280
----------	----------	----------

972.5321	973.7944	1035.1036
----------	----------	-----------

1068.3393	1129.2698	1154.1645
-----------	-----------	-----------

1223.8342	1231.5469	1308.6237
-----------	-----------	-----------

1319.1067	1326.6826	1377.9063
-----------	-----------	-----------

1484.9848	1490.4453	1509.6503
-----------	-----------	-----------

1679.7423	2995.1374	2996.6206
-----------	-----------	-----------

3034.5877	3043.4115	3054.4307
-----------	-----------	-----------

3089.8961	3165.1862	3190.1907
-----------	-----------	-----------

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

End

GroundEnergy[kcal/mol] 62.38

End

!-----c10h15_R1_ts1-----

Barrier R1_ts1 R1 R1-1

RRHO

```

Geometry[angstrom]    25
C   -1.1396940856      0.146710467      2.19138368
C   -0.5405329124     -0.9735279137      2.7406373323
C    0.821450804     -1.0846498232      1.001913463
C   -0.0649822151     -1.0738123242     -0.2260656271
C   -0.7397068978      0.3529198479     -0.1866861827
C   -0.3019530741      0.9261496646      1.1999861225
C    1.1327310727      0.3623542589      1.3196619279
C    0.6993132409     -1.1314016661     -1.5848308876
C   -0.2295766933      1.0939389902     -1.4421502744
C    0.0588361399     -0.0312073693     -2.4493105917
H   -2.218320284      0.1722644622      2.0595928128
H   -1.1658332652     -1.7949176204      3.0867076243
H    0.416791857     -0.9275283151      3.2466471562
H    1.5382939528     -1.8837949015      1.1667965226
H   -0.8105360563     -1.871963663      -0.1933812794
H   -1.828533806      0.2730048885     -0.2373849986
H   -0.3863413145      2.0143600142      1.2582263902
H    1.8001106278      0.8207233342      0.5789321462
H    1.5881999516      0.5195698785      2.3003109654
H    0.6487045195     -2.1217414781     -2.0437941232
H    1.7596593681     -0.9044153712     -1.4292608436
H    0.6970122725      1.6356626175     -1.2224512221
H   -0.9510147447      1.8273803389     -1.8112397773
H   -0.8816510399     -0.3931191147     -2.8803453516
H    0.6962225821      0.285611798      -3.279384984
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm]  664.5938
WellDepth[kcal/mol]  35.85
WellDepth[kcal/mol]  23.66
End
Frequencies[1/cm]  68
128.2243           166.4117
273.2941           301.4062           356.0210
370.2903           487.2404           536.2461
553.3203           608.3972           663.4828
684.3323           720.8220           764.8083
785.9030           852.5215           886.9098
887.9765           898.8287           906.2843
915.2520           928.4011           949.6449
953.6268           980.9753          1000.9521
1025.5896          1030.4029          1044.8893
1061.4353          1089.4838          1130.0213
1163.3844          1188.4805          1188.8156
1223.6238          1244.6009          1253.5657
1264.7300          1289.4922          1299.8170
1313.0270          1322.5093          1330.2690
1338.8274          1341.5861          1362.5454
1404.9019          1491.2998          1494.7892

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1502.8503          1514.9404          1541.4663
3006.5978          3018.5482          3023.4991
3026.9616          3040.8144          3052.2357
3060.5055          3069.3484          3071.0426
3075.2327          3083.3869          3101.9753
3134.0637          3151.2074          3170.0240
ZeroEnergy[kcal/mol] 35.85
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-1_ts1-----
Barrier      R1-1_ts1  R1-1  R1-1_i1
RRHO
Geometry[angstrom] 25
C -1.3640621808    1.2316621783    0.7273362271
C -2.1215885296    2.0580177071    1.4825906983
C -0.3549883989    -2.3376268114    1.3385284768
C 0.7669555473     -1.8891036923    0.4518802882
C 0.7611913792     -0.2875311223    0.5085225268
C -0.4899122325     0.2122599207    1.2410074836
C -1.5431220309     -1.6500189009    1.1888308597
C 0.6179396491     -2.2466249625    -1.063526635
C 0.9267358314     0.1443058244    -0.9650046014
C 0.2246954126     -0.945134498     -1.7853152766
H -1.4518842427     1.3162149548     -0.3536395157
H -2.7920677801     2.7807238735     1.033666539
H -2.0829146605     2.0283834209     2.5670131757
H -0.1229265578     -2.8269886042     2.2797510252
H 1.7179154078      -2.276892992     0.82218441
H 1.6247377389      0.0550360744     1.0870937756
H -0.369189246      0.2443360863     2.3206537235
H -2.3213675872     -1.7138399113     1.9437196335
H -1.9090321492     -1.3990333235     0.1994043244
H -0.1049042835     -3.0509027006     -1.2151059565
H 1.5792050899      -2.6011084125     -1.4480371819
H 1.9948692387      0.1429578482     -1.2089773422
H 0.5609991554      1.1527589798     -1.1668285232
H -0.8609035666     -0.8026017348     -1.7587261659
H 0.5208189961      -0.9420162022     -2.8376569689
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 650.9231
WellDepth[kcal/mol] 28.2
WellDepth[kcal/mol] 22.7
End
Frequencies[1/cm] 68
43.9831          118.7931
175.6410          204.7367          239.8507
280.4732          339.6892          397.6519

```

441.7956	513.5470	538.8510
621.1035	643.7491	683.4036
752.9376	766.8800	793.8729
821.7193	862.5832	878.3282
898.2919	907.7442	918.5771
948.4009	964.7313	994.2386
1006.4871	1015.2735	1026.8098
1075.8824	1088.8287	1093.3597
1141.0608	1180.5289	1188.7404
1227.3523	1254.8892	1273.5445
1286.5279	1302.9528	1314.5861
1319.0362	1334.2764	1349.4332
1358.9079	1370.0891	1412.5063
1465.1764	1491.4196	1500.2567
1515.4203	1542.1890	1594.5756
3018.9224	3028.9698	3032.4117
3035.8231	3065.4175	3072.1348
3085.4352	3089.3066	3120.6366
3122.2453	3131.0236	3134.3670
3148.2646	3195.5864	3218.8564

ZeroEnergy[kcal/mol] 40.39

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R1-1_ts3-----

Barrier R1-1_ts3 R1-1_i1 R1-1_i3

RRHO

Geometry[angstrom] 25

C	-1.1307218241	1.5860626191	1.0569678475
C	-2.0084624449	2.0648062885	1.9734961693
C	-0.0741649995	-2.0393794526	1.2697649687
C	0.9768147257	-1.5763270171	0.3986620216
C	1.1298802478	0.6266023073	0.4726558811
C	0.1947020998	1.1629577425	1.3587921054
C	-1.3367735807	-2.3656673485	0.9312710074
C	0.8969056597	-1.6633189985	-1.1025879223
C	1.0757141854	0.7907353418	-1.0311508849
C	1.6291387616	-0.4636578284	-1.7166980852
H	-1.4583380959	1.5326555155	0.0222418419
H	-3.0044030385	2.3838910831	1.6926730943
H	-1.7418803152	2.144332479	3.0224603745
H	0.1886135358	-2.0921328187	2.3247348994
H	1.9789719374	-1.7036123597	0.8004880889
H	2.1400502907	0.5544053434	0.8676979057
H	0.4760788135	1.198147771	2.4093373009
H	-2.0513750611	-2.6745930221	1.6843278645
H	-1.6921408542	-2.3442783728	-0.0923199209
H	-0.1461409417	-1.6525432632	-1.432639183
H	1.3291215214	-2.6089530357	-1.4549578574
H	1.6493771522	1.6791124536	-1.321280953
H	0.0479293448	0.9598056687	-1.3641974189

```

H 1.5035020189 -0.4214406699 -2.8025114368
H 2.7052388611 -0.5475984264 -1.5215327086
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 537.4401
WellDepth[kcal/mol] 22.7
WellDepth[kcal/mol] 11.23
End
Frequencies[1/cm] 68
43.4661 62.2157
106.5508 157.2986 193.0092
215.8916 255.1222 293.7953
300.7399 369.4621 449.6244
491.5284 576.3648 622.9125
637.8363 654.2039 772.5589
825.2328 852.7059 868.1651
884.8445 886.2849 893.5048
907.5659 941.3710 966.4314
982.0019 1016.1710 1024.4228
1025.6341 1051.3737 1084.9769
1117.1813 1181.9638 1188.1692
1222.1696 1242.5486 1262.9229
1308.5893 1322.6689 1329.0741
1340.5433 1360.5783 1384.3229
1430.7677 1447.7119 1459.1968
1476.0067 1483.4262 1501.4150
1503.9442 1575.5921 1622.3799
3001.6979 3012.8442 3020.7484
3054.3938 3060.9656 3075.1833
3111.2241 3118.6733 3128.5302
3133.1676 3138.5285 3144.4349
3146.1872 3223.9222 3224.2496
ZeroEnergy[kcal/mol] 40.39
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-1_ts7-----
Barrier R1-1_ts7 R1-1_i3 R1-1_p2
RRHO
Geometry[angstrom] 25
C 1.9474681989 2.9426297824 1.3452935074
C 2.723733019 3.8768880353 1.9077977202
C -2.4908970695 -2.5302523013 -1.17799855
C -1.7802806385 -2.1508499192 0.0348657336
C 0.7795048015 2.0510595116 -0.6851791469
C 1.5610713096 2.9463769597 -0.0568089033
C -1.9552522021 -2.976646604 -2.3249827659
C -0.4632226579 -2.3458036493 0.2924762729
C 0.1402350894 0.8121390318 -0.1007408229

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C 0.7979869042 -0.416443381 -0.6581339234
H 1.5839015888 2.128414476 1.9659051644
H 2.9910331034 3.8383916928 2.9569263611
H 3.1152441196 4.7099102654 1.33207098
H -3.5722541983 -2.4216299584 -1.133501469
H -2.3754329637 -1.6385984055 0.7862460531
H 0.5991150766 2.1965016632 -1.7476019712
H 1.9540983884 3.7731443248 -0.6451784873
H -2.5813622145 -3.2402895187 -3.1686729482
H -0.8851391274 -3.0916767313 -2.4599103441
H 0.1566842285 -2.9633727098 -0.3459211571
H -0.0492498226 -2.0915463065 1.259641387
H -0.9257975262 0.8050056613 -0.3565668883
H 0.2060310088 0.8178317991 0.9899346765
H 0.590890577 -0.6926545002 -1.6861619634
H 1.7740950069 -0.6976882181 -0.2766215153
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 258.7853
WellDepth[kcal/mol] 36.33
WellDepth[kcal/mol] 3.11
End
Frequencies[1/cm] 68
16.0327 29.4326
45.9836 72.7112 85.3560
118.4090 135.2459 214.4060
234.2011 270.4696 298.6079
384.1237 445.0490 452.1951
538.0370 602.2255 616.0759
669.5135 722.7945 753.3246
802.6071 819.1056 887.6977
892.1312 906.3213 911.9198
928.8068 977.8777 985.0370
996.4014 1023.2235 1036.5295
1055.7355 1067.6182 1081.4590
1110.4807 1186.5560 1272.9593
1283.7810 1294.2482 1299.3176
1328.4173 1337.6664 1397.5868
1437.0707 1457.2604 1461.1353
1469.9582 1485.4045 1573.0830
1646.6982 1660.0808 1694.9563
3017.0351 3072.5093 3118.8913
3120.5463 3126.5286 3131.0619
3137.5229 3143.7133 3144.0750
3150.2123 3150.8158 3218.7855
3219.1352 3220.9905 3231.6293
ZeroEnergy[kcal/mol] 65.49
ElectronicLevels[1/cm] 1
0 2
End

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!-----
!-----c10h15_R1-1_ts2-----
Barrier      R1-1_ts2  R1-1  R1-1_i2
RRHO
Geometry[angstrom]  25
C  -1.452471065    1.1951706471    0.712890387
C  -1.8965239129    2.2039139557    1.4593644731
C  -0.3687679744    -2.3733244092    1.2739252037
C  0.7342948557     -2.3574138512    0.4404873174
C  0.7386338502     -0.092531061     0.5912805878
C  -0.6514398781    0.0276007751     1.2204432953
C  -1.4286171067    -1.3406241808    1.0591246172
C  0.7324030929     -2.3097399764    -1.0894707678
C  0.9693948508     0.149624417     -0.8731149677
C  0.3108191003     -0.96470907     -1.7004542032
H  -1.6944164342    1.1857681656     -0.3488752096
H  -2.4843116866    3.0106202206     1.0354990827
H  -1.6873133193    2.2590185869     2.5236734605
H  -0.2359377166    -2.7426808109     2.2878288267
H  1.6260123575     -2.8367719806     0.8420801431
H  1.559268106      0.1677774109     1.2525363382
H  -0.5032164289    0.167746545      2.2960799709
H  -2.2430817845     -1.39797132      1.7843603412
H  -1.8778317933     -1.3968567403     0.0627824065
H  0.1032068553     -3.119514957     -1.4756335481
H  1.7514943623     -2.5319949431     -1.422195837
H  2.0470960181     0.1560289421     -1.067595008
H  0.5922348458     1.1330824459     -1.1870653381
H  -0.7768109083     -0.8548123923     -1.6791270523
H  0.6067317138     -0.9077214192     -2.7528855194
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  515.1491
WellDepth[kcal/mol]  31.79
WellDepth[kcal/mol]  12.91
End
Frequencies[1/cm]  68
66.6261          83.6874
173.2062          234.2236          279.4933
308.5388          310.3799          400.4828
438.3126          449.2515          507.1312
620.1234          645.5209          674.0061
703.0888          742.3627          776.1089
806.3375          863.8372          887.6725
906.7967          938.8350          942.5667
950.6920          961.0154          994.0190
1009.4646         1033.5803         1061.8030
1073.6082         1121.5794         1146.5953
1156.5324         1176.9699         1223.6719
1247.3258         1266.1616         1268.3097

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1314.7337          1318.8185          1329.9154
1343.4547          1357.6230          1365.4921
1382.0608          1409.6831          1455.2556
1480.7244          1488.2228          1493.6945
1505.9986          1514.2635          1694.1260
2984.5149          3019.0360          3027.8842
3032.2446          3039.9550          3040.5654
3048.2282          3074.2296          3086.4084
3107.2168          3115.6580          3125.8850
3139.0144          3148.4430          3206.2777
ZeroEnergy[kcal/mol]  43.98
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-1_ts4-----
Barrier      R1-1_ts4  R1-1_i2  R1-1_p1
RRHO
Geometry[angstrom]  25
C  1.8777059586  -0.2647129638  -0.5966495228
C  3.0261955085  -0.1224044948   0.0206122288
C  -2.0001048195  1.9233908754  -0.1774268628
C  -3.1871027983  1.371251976   0.0776580847
C  -0.6316389682  -0.823839848   0.9621719762
C  -0.1377466746  0.3652259689   0.5387028264
C  -0.7077981452  1.2287010629  -0.5730601664
C  -3.6477648172  -0.0646769728   0.0223613384
C  -1.6575644547  -1.7244792404   0.3272815002
C  -2.7361493841  -1.1375380959  -0.6009628487
H  1.6268688532  -0.6785231469  -1.5662913377
H  3.9729530331  -0.4225896415  -0.4352484462
H  3.1004881394  0.3052637264   1.0187656816
H  -1.9292783689  3.0023568275  -0.0639798293
H  -3.9807934425  2.0558123679   0.3740361062
H  -0.1675309233  -1.2468439493   1.850258091
H  0.5368162266  0.8784581437   1.2169063597
H  0.0330517969  1.9876520267  -0.8304073391
H  -0.849194591  0.6369995031  -1.4787601221
H  -4.5963896535  -0.065028386  -0.5304368479
H  -3.9233147882  -0.3766001719   1.0406218146
H  -2.1705787018  -2.2535983808   1.1408228682
H  -1.1259395046  -2.5168882701  -0.2229226864
H  -2.3024795821  -0.7657536573  -1.5310525987
H  -3.3756678985  -1.9764062591  -0.896817268
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  281.0499
WellDepth[kcal/mol]  38.0
WellDepth[kcal/mol]  2.87
End

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Frequencies[1/cm]  68
28.4627          33.6663
92.5931          108.3604          162.5938
214.5593         263.6093         268.6048
296.1234         319.0901         382.8526
410.6105         530.4128         644.6367
675.0951         701.6348         736.1119
774.8424         792.2905         830.8184
877.7884         882.5240         883.8908
928.6193         932.3685         950.2636
999.4685         1005.2978        1020.6269
1032.4613        1085.1354        1095.8898
1112.8979        1176.6981        1213.1016
1257.7618        1277.0483        1290.9622
1300.6459        1331.5287        1377.4396
1395.5638        1396.7746        1397.8368
1421.5216        1429.8637        1467.2173
1477.4769        1492.7816        1529.7712
1600.1364        1643.5218        1720.8360
2964.6749        2982.8221        3005.0197
3008.1107        3032.2931        3046.9633
3062.7687        3083.1987        3099.3154
3107.6782        3124.3667        3129.2252
3138.9063        3152.6219        3187.6311
ZeroEnergy[kcal/mol]  69.07
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-1_ts5-----
Barrier          R1-1_ts5  R1-1_i2  R1-1_i4
RRHO
Geometry[angstrom]  25
C  2.0308749597 -0.4942830104 -0.2845830055
C  3.2221289379 -0.047997995  0.1026186458
C -1.3053015058  1.4627645791 -0.4630799551
C -2.5377824702  1.0309493877 -0.1783158919
C -0.1295555365 -1.0563376166  0.8510545105
C  0.7045742918  0.034963931  0.2084078489
C -0.0877548091  0.7172439848 -0.9536246278
C -3.1981114986 -0.3253666482 -0.2640793598
C -0.6312277613 -2.1231449147  0.1741614427
C -2.530410682 -1.4529415714 -0.9877205444
H  1.9783091696 -1.3006871765 -1.0141706906
H  4.1422154024 -0.4665371086 -0.2899303569
H  3.3210014316  0.7516276039  0.8309758991
H -1.1233498938  2.5174303761 -0.2633236262
H -3.2186711849  1.7870894649  0.2109117813
H -0.4190764833 -0.9084085698  1.8866920696
H  0.9105143892  0.8020331392  0.9618133714
H  0.5829882662  1.4248058098 -1.4498070047
H -0.3425137572 -0.0426895941 -1.6934596356

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H  -4.1899794818   -0.1623771988   -0.7227030411
H  -3.435152159    -0.6424104668    0.7621330903
H  -1.1603851341   -2.9025800697    0.7090300561
H  -0.2421030464   -2.4071606401   -0.7970341682
H  -2.0995803494   -1.2479800286   -1.9614849527
H  -3.016832095    -2.4207066672   -0.9116768552
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  401.5198
WellDepth[kcal/mol]  27.96
WellDepth[kcal/mol]  13.14
End
Frequencies[1/cm]  68
42.9841          83.4346
134.1007         171.4448         206.4295
238.3241         259.0051         300.3278
350.0717         358.0148         390.8058
489.1419         541.8473         565.3645
666.7538         677.1833         702.5840
721.3396         779.0742         810.0251
845.6208         879.0969         919.1460
938.7559         947.0370         964.3985
984.5869         1004.6745        1012.6713
1025.9611        1037.1816        1064.6975
1069.2215        1116.7847        1156.9968
1216.0301        1243.6051        1278.5313
1296.7110        1309.7698        1321.6989
1337.5899        1360.6526        1385.4458
1427.2526        1433.4729        1448.2079
1453.3636        1467.9013        1503.8261
1572.7018        1698.0405        1718.6690
2923.8095        2985.9954        3033.9854
3044.0004        3092.3749        3102.5238
3115.6061        3117.6633        3126.5803
3126.6870        3132.6905        3152.8942
3202.2759        3205.9255        3214.6449
ZeroEnergy[kcal/mol]  59.03
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-1_ts9-----
Barrier      R1-1_ts9  R1-1_i4  R1-1_p3
RRHO
Geometry[angstrom]  25
C  2.8812577957   1.2166874362   0.8025257094
C  2.8615928943   2.2744950518   1.6080887507
C  0.4519758512   1.305581317    -1.0883516971
C  -0.8212748457   1.4112208034   -1.3945692306
C  2.3983431155   -1.1599535153   1.2195391953

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C	1.8107355442	0.148732061	0.727928603
C	1.1895475855	0.0543616698	-0.6851166032
C	-2.4814750033	-0.2673928403	-1.4090626968
C	2.5638501387	-2.2823632554	0.5248956738
C	-2.0184990887	-1.5067466583	-1.1317716616
H	3.7315786515	1.0639132257	0.1387777896
H	3.6712699126	2.9957605256	1.6192906843
H	2.0331266783	2.4578869735	2.2856999627
H	1.058063466	2.2188351783	-1.1125264267
H	-1.4071026528	2.2731387788	-1.6906583811
H	2.7320155996	-1.1317437875	2.255193805
H	1.0119284634	0.430987617	1.4262380301
H	1.990050656	-0.1390650344	-1.4109903227
H	0.5044467061	-0.7935022734	-0.7239603432
H	-2.6510050577	0.0438534148	-2.4327771978
H	-2.9550534279	0.3318395106	-0.640745723
H	3.0118667536	-3.1583126781	0.9806083488
H	2.2623376632	-2.3788369847	-0.5119822236
H	-1.9543972224	-1.8749396924	-0.1140008064
H	-1.649631177	-2.161993844	-1.9129492388
Core RigidRotor			
SymmetryFactor 1.0			
End			
Tunneling Eckart			
ImaginaryFrequency[1/cm] 305.9604			
WellDepth[kcal/mol] 36.81			
WellDepth[kcal/mol] 4.78			
End			
Frequencies[1/cm] 68			
25.8772	38.1801		
51.4650	80.2195	101.4417	
123.8336	135.2274	203.9810	
229.6986	282.7022	315.4614	
352.0284	384.3106	416.0896	
477.8731	572.8058	627.9247	
678.2769	696.7289	828.5154	
833.3533	869.1084	873.7733	
890.1402	925.9760	942.8087	
947.1612	951.9558	976.0868	
1002.0630	1022.2787	1035.4278	
1040.3762	1072.1427	1135.4133	
1151.5897	1233.5874	1239.7237	
1265.7818	1292.2602	1310.5240	
1319.9138	1321.9611	1339.0169	
1361.1448	1447.8588	1452.0316	
1466.3969	1487.8117	1587.4741	
1674.2341	1691.7250	1703.8476	
2999.6495	3012.8903	3020.5281	
3098.5438	3114.8226	3122.8562	
3127.7362	3130.1556	3139.9692	
3140.6437	3187.5059	3205.3950	
3208.3910	3216.1251	3232.9291	

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ZeroEnergy[kcal/mol]  82.70
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-1_ts6-----
Barrier      R1-1_ts6  R1-1_i2  R1-1_i5
RRHO
Geometry[angstrom]  25
C  1.6755580022  -0.6568801542  -0.5212032203
C  2.9317869171  -0.249783027  -0.7199597966
C  -1.5055151024  1.726476153  -0.3010721538
C  -2.6397743163  0.9956262408  -0.2134495321
C  -0.3270640452  -0.7617559417  1.0027111236
C  0.7438868502  -0.0568430821  0.4472502897
C  -0.2275824987  1.3384551735  -0.8473330984
C  -2.9772136076  -0.3950649177  -0.7035400922
C  -1.074931  -1.8741549271  0.3276317927
C  -1.8739163557  -1.4446694683  -0.9324640647
H  1.3009953572  -1.4909747652  -1.1101405534
H  3.5772701754  -0.7327643897  -1.4439289939
H  3.3571920864  0.5770174433  -0.1590595499
H  -1.534774769  2.7042760051  0.1760364231
H  -3.4849343921  1.4900365886  0.261410582
H  -0.7891380105  -0.3321346465  1.8847530976
H  1.1973572799  0.6911707684  1.0929825698
H  0.5505884047  2.0940718262  -0.86228407
H  -0.2044757954  0.6914524095  -1.7134600852
H  -3.5408157427  -0.2923798097  -1.6432973483
H  -3.7018279653  -0.8184561154  0.0045807848
H  -1.7702380118  -2.3234115591  1.0442434641
H  -0.3886207756  -2.6750577253  0.0253152878
H  -1.1820213314  -1.1094373592  -1.7074936647
H  -2.3582053533  -2.3412277201  -1.3363681918
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  603.4337
WellDepth[kcal/mol]  19.84
WellDepth[kcal/mol]  20.56
End
Frequencies[1/cm]  68
63.9966          104.2262
156.2421          192.2150          202.4747
261.9869          279.3658          291.5297
381.7867          396.1512          444.8852
463.4423          613.0476          647.9557
676.6856          699.3911          724.1216
757.3572          772.0809          831.3382
865.3026          895.0771          917.4445
921.7855          936.5037          981.0437

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990.5487          1007.4817          1033.9109
1037.2907          1060.0779          1070.8989
1136.4581          1152.5032          1207.8369
1226.8443          1247.4900          1284.0002
1303.7494          1321.6875          1349.9816
1370.9454          1388.7210          1395.1659
1429.5588          1453.5967          1470.1254
1484.3160          1490.7449          1493.6896
1510.5371          1629.1626          1681.7219
2974.0229          3001.6717          3005.2833
3026.8129          3045.7992          3088.9327
3108.2072          3121.1129          3128.5322
3130.7798          3137.4558          3139.1110
3165.4393          3214.1873          3220.9589
ZeroEnergy[kcal/mol] 50.91
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-1_ts12-----
Barrier      R1-1_ts12  R1-1_i5  R1-1_p2
RRHO
Geometry[angstrom] 25
C 1.9572527708 -2.0339343366 1.2835668777
C 2.9015924438 -1.9336329278 2.2263526923
C -2.9932309819 1.8020020804 0.0967670143
C -2.1162541769 0.8089615663 0.6965045137
C 0.8331798498 -1.0825957047 -0.7445551916
C 1.7501841698 -1.0453375809 0.2349566096
C -4.068795917 1.5729207593 -0.673974771
C -2.3522108514 -0.525575884 0.7844423463
C -0.192342711 -2.1516266972 -1.0093643283
C -1.5655885427 -1.6169308841 -1.2885983729
H 1.3050224908 -2.9027400726 1.293905282
H 3.0245390566 -2.6905808661 2.9915521062
H 3.5821839264 -1.0884088024 2.2588212132
H -2.7220105824 2.8373957354 0.2916857824
H -1.169970991 1.1819192584 1.0782083045
H 0.8176929685 -0.2550938884 -1.4506950163
H 2.4232475366 -0.1908927086 0.2637779168
H -4.6621192828 2.3911528833 -1.0638377384
H -4.3864929692 0.5711064176 -0.942333119
H -3.326582869 -0.9425408948 0.560512292
H -1.6662358896 -1.1646470617 1.3243523262
H -0.2294132888 -2.8824983795 -0.1962661283
H 0.1432597776 -2.7276714264 -1.8934373245
H -1.6635506478 -0.7206503904 -1.8904164275
H -2.3813352892 -2.3285701945 -1.3640308592
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart

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ImaginaryFrequency[1/cm] 307.803
WellDepth[kcal/mol] 48.76
WellDepth[kcal/mol] 16.73
End
Frequencies[1/cm] 68
14.9693 21.6919
51.6456 59.6674 110.1147
120.5241 145.3301 194.3342
243.3131 289.5256 307.2377
375.2592 417.2067 481.6282
531.5640 610.4226 618.6582
672.6389 703.4769 754.7518
801.0691 856.5184 871.4892
889.7887 907.8396 927.3440
933.1342 944.2910 984.7821
996.1942 1022.9908 1038.5488
1062.0151 1069.0981 1082.3024
1110.8986 1180.9899 1207.0449
1287.8822 1293.5543 1316.2581
1335.0123 1344.8002 1403.2131
1433.7112 1455.1916 1456.6915
1461.9179 1474.6811 1565.2083
1655.0921 1656.7402 1707.3384
2893.4500 3050.3600 3118.4649
3120.7012 3125.9593 3130.9700
3136.5451 3140.8878 3145.7070
3148.8848 3152.0713 3218.1731
3219.2075 3219.5419 3235.0526
ZeroEnergy[kcal/mol] 79.11
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1_ts2-----
Barrier R1_ts2 R1 R1-2
RRHO
Geometry[angstrom] 25
C -0.7676505811 0.3290987009 2.4374626215
C -0.2415955201 -1.0855023016 2.3450419919
C 0.7161767057 -0.9926142315 1.1248722367
C -0.045792524 1.1412146299 1.5952975779
C 1.2622850317 0.442520793 1.2629689195
H -1.6789378222 0.6050580805 2.952859964
H -1.0319013009 -1.8327941279 2.2031193463
H 0.3065961244 -1.3810410191 3.2525354592
H 1.4800536751 -1.7748869967 1.1252302976
H -0.185220963 2.2127647126 1.5113969782
H 1.7578377928 0.8154885317 0.3647967199
H 1.9729022027 0.5275080584 2.0941922158
C -0.0974491922 -0.9883458058 -0.1994722484
C -0.8521163622 0.337197213 -0.331287128
C 0.7822027667 -1.0691969768 -1.4782656417

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C  -0.4035476977    1.0499603684   -1.5896343515
C  0.1395535423    -0.0917475655   -2.4806310765
H  -0.798993998    -1.8312743326   -0.1835849438
H  -1.9082716803    0.3567593585   -0.0880803211
H  0.8478402826    -2.0883235958   -1.8671087534
H  1.8051241258    -0.7492439376   -1.253292694
H  0.4070843486    1.7621290418   -1.3782586496
H  -1.2057359203    1.6212465042   -2.0640987819
H  -0.6948072295    -0.5790736063   -2.9961126197
H  0.8396871929    0.2554685042   -3.2459391189
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  484.9887
WellDepth[kcal/mol]  25.33
WellDepth[kcal/mol]  12.9
End
Frequencies[1/cm]  68
120.0126          139.6449
240.9716          283.2947          315.7284
360.6503          454.0442          518.7058
566.8263          637.2880          662.0888
750.6497          779.5005          788.3011
816.2019          849.4403          878.5888
893.9539          900.7648          908.6138
917.5793          932.5279          942.7496
963.7376          976.0064          1013.4297
1021.6001         1030.3680          1038.6895
1091.4617         1095.1501          1134.5516
1158.6235         1164.9436          1192.5575
1220.7378         1233.1818          1273.9413
1289.0946         1295.1873          1299.9631
1305.5976         1315.8564          1333.0834
1347.8889         1350.9794          1366.3519
1460.7507         1480.1647          1485.3984
1491.3172         1503.2497          1514.7823
2966.6156         2974.5730          3003.0466
3016.1437         3019.3569          3024.2677
3027.4625         3060.4407          3062.6475
3066.7513         3078.1294          3085.3276
3161.4858         3175.3770          3196.9584
ZeroEnergy[kcal/mol]  25.33
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-2_ts1-----
Barrier      R1-2_ts1  R1-2  R1-2_p6
RRHO
Geometry[angstrom]  25
C  -2.526136    0.425442    0.691845

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C  -2.103829    1.223089   -0.288402
C  -1.285468    0.472432   -1.315615
C  -1.11712     -0.896866   -0.683917
C  -2.064182    -1.001981    0.497901
C   0.955039   -1.147941    0.146288
C   1.086548   -0.193017    1.325504
C   1.754556    1.055687    0.703543
C   2.522157    0.527676   -0.535045
C   1.852967   -0.789738   -0.828031
H  -3.142815    0.735459    1.527839
H  -2.327143    2.280704   -0.371537
H  -1.823859    0.413582   -2.2756
H  -0.330698    0.959862   -1.547983
H  -1.015091   -1.753004   -1.341759
H  -1.594361   -1.420514    1.399182
H  -2.916738   -1.665705    0.281112
H   0.644921   -2.17489    0.301861
H   0.141743    0.04284    1.818757
H   1.736686   -0.647823    2.084689
H   0.981304    1.76033    0.387877
H   2.402513    1.580976    1.408282
H   2.499699    1.230069   -1.376713
H   3.586703    0.368564   -0.305802
H   2.082598   -1.385227   -1.704285
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  485.122
WellDepth[kcal/mol]  27.72
WellDepth[kcal/mol]  7.88
End
Frequencies[1/cm]  68
38.9488          80.7356
116.9902         147.8121         197.8795
210.6207         279.2349         395.8675
409.9720         616.0001         684.4384
705.2614         714.8557         764.0990
791.8734         801.1901         833.4047
875.0998         883.6015         898.2456
905.0124         921.7804         923.6357
950.4524         965.7183         971.0196
980.0515         1009.3905        1033.0927
1052.1492        1060.9570        1103.2830
1127.1499        1136.5748        1149.0503
1171.1798        1215.9743        1233.1271
1260.8452        1301.5349        1306.0190
1314.6946        1320.2581        1322.9855
1368.0034        1379.7398        1468.2946
1472.7549        1476.0142        1487.2371
1501.2962        1512.9790        1674.0755
2950.6524        2953.2981        2967.2338

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2984.3229          2997.5918          3011.7484
3015.1976          3050.1292          3078.9249
3090.1590          3152.6147          3158.0150
3167.1757          3179.8892          3191.8853
ZeroEnergy[kcal/mol] 40.15
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-2_ts2-----
Barrier          R1-2_ts2  R1-2  R1-2_i2
RRHO
Geometry[angstrom] 25
C -3.100763  0.465674  -0.119753
C -2.902683  -0.581121  0.678856
C -1.482312  -1.088782  0.613256
C -0.891348  -0.348563  -0.623655
C -1.84853  0.85454  -0.866938
C 0.602941  0.007048  -0.564065
C 1.028223  1.003445  0.577484
C 2.531924  1.018502  0.718813
C 2.872774  -0.881909  -0.46046
C 1.534071  -1.15757  -0.360384
H -4.032878  1.012551  -0.208806
H -3.650134  -1.013209  1.335058
H -1.428548  -2.176654  0.502934
H -0.947616  -0.849448  1.541829
H -1.015242  -1.024376  -1.477175
H -1.443335  1.793904  -0.468987
H -2.023752  1.025089  -1.934483
H 0.862431  0.493107  -1.515394
H 0.571494  0.683888  1.518307
H 0.645823  2.007389  0.364807
H 2.970653  0.80746  1.686974
H 3.098033  1.715331  0.108806
H 3.617468  -1.561856  -0.058289
H 3.238699  -0.205496  -1.225408
H 1.192619  -1.998942  0.236683
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 560.274
WellDepth[kcal/mol] 34.65
WellDepth[kcal/mol] 17.2
End
Frequencies[1/cm] 68
57.7723          76.4703
104.8602          183.0445          226.1314
296.8709          351.9557          393.1336
435.8898          492.9231          526.0631
532.7703          671.3626          686.4991

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710.1363	769.5487	782.2775
816.7882	825.4545	874.1388
905.7407	922.3368	930.0974
948.3452	960.6113	976.1103
978.9387	1003.7580	1033.2858
1047.2314	1065.6872	1121.4748
1135.4704	1153.7636	1166.1954
1207.2604	1235.2088	1263.1980
1273.6296	1293.8035	1301.8724
1311.6790	1334.8927	1344.6232
1368.4344	1383.2286	1433.4128
1463.7863	1487.8140	1493.7316
1498.0347	1550.3749	1683.0340
2979.5169	3000.7984	3003.0762
3014.4220	3025.9762	3039.0673
3047.4368	3067.6014	3116.4490
3121.0002	3142.1268	3163.3705
3188.2322	3193.8946	3212.1403

ZeroEnergy[kcal/mol] 47.08

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R1-2_ts9-----

Barrier R1-2_ts9 R1-2_i2 R1-2_p1

RRHO

Geometry[angstrom] 25

C	2.726958	-0.314631	-0.796056
C	2.870608	0.397044	0.31952
C	1.663428	0.313993	1.218214
C	0.737329	-0.728153	0.517335
C	1.395388	-1.019291	-0.870827
C	-0.729984	-0.345603	0.490435
C	-2.979985	-1.362291	0.250699
C	-1.684047	-1.257734	-0.100497
H	3.465317	-0.38186	-1.58753
H	3.743137	0.991586	0.566807
H	1.176625	1.291439	1.321936
H	1.926058	-8.01E-4	2.234051
H	0.800966	-1.655822	1.102514
H	1.510524	-2.093732	-1.049425
H	0.795094	-0.634965	-1.703421
H	-1.073168	0.130839	1.405242
H	-3.650899	-2.048314	-0.252523
H	-3.398503	-0.763918	1.053667
H	-1.320859	-1.882867	-0.915343
C	-0.86516	1.406185	-0.74955
C	-1.795723	2.275576	-0.224358
H	-1.127606	0.841874	-1.636667
H	0.187759	1.65005	-0.661592
H	-1.524177	3.005048	0.53068
H	-2.84908	2.186352	-0.463312

```

Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  577.7169
WellDepth[kcal/mol]  21.98
WellDepth[kcal/mol]  14.58
End
Frequencies[1/cm]  68
22.6097           42.2057
84.3435           121.9210           160.3356
196.0448          235.7784           269.0698
348.1616          372.0574           388.3232
424.0016          537.2306           648.9702
671.0190          711.0840           782.3567
787.9810          809.6210           819.4824
867.9568          890.3899           922.5378
944.5006          963.2198           979.8153
983.1185          988.1211           997.8548
1020.9363         1035.3562           1055.7890
1114.0452         1132.9056           1171.8534
1185.9915         1203.4466           1242.4633
1253.6470         1290.0425           1297.7857
1304.8666         1314.7170           1335.2273
1351.8070         1377.8216           1459.9630
1462.0101         1494.2580           1499.1271
1543.8565         1616.3622           1687.2819
2972.7744         3010.7329           3019.0286
3036.0688         3042.6651           3111.9439
3123.7545         3129.0292           3130.5162
3131.7065         3163.6197           3188.2458
3198.9083         3216.8011           3225.6748
ZeroEnergy[kcal/mol]  51.86
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-2_ts3-----
Barrier      R1-2_ts3  R1-2  R1-2_i3
RRHO
Geometry[angstrom]  25
C  -3.1382404148   -0.4598747144   -0.0237284596
C  -2.9872981423    0.8075444606   -0.4031938623
C  -1.5832633846    1.3089264298   -0.1591888017
C  -0.9769565475    0.2241820772    0.7729299736
C  -1.8621916382   -1.0355472738    0.5418902936
C   0.5094837286   -0.0157573039    0.6502083474
C   1.3613389572   -1.2136331041   -1.0428134226
C   2.7447609199   -0.9232815743   -0.5200577012
C   2.8189148448    0.5517405949   -0.0190072066
C   1.4265694606    0.9719661004    0.3729807937
H  -4.0466377797   -1.0406999697   -0.1379221772

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H   -3.7545957623    1.4131227834   -0.8724488744
H   -1.5570141896    2.3068889615    0.2896631872
H   -1.0275632374    1.376815511   -1.1040743392
H   -1.1697577841    0.5473240279    1.8051452339
H   -1.3964330329   -1.7207016729   -0.1775510385
H   -2.0177501973   -1.6053697801    1.4639602365
H    0.8522944304   -0.8985960487    1.1870918271
H    1.0308817427   -0.6701964563   -1.9234245947
H    0.9828948548   -2.229393085   -0.9733360373
H    3.5179650962   -1.1008595197   -1.2781563046
H    2.9688863354   -1.6068689951    0.3054002107
H    3.175125335    1.2075051726   -0.8213014021
H    3.5508892441    0.6463207945    0.7926163149
H    1.0914361608    1.9722295845    0.1177728036
Core   RigidRotor
SymmetryFactor   1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm]   533.6033
WellDepth[kcal/mol]   34.18
WellDepth[kcal/mol]   16.97
End
Frequencies[1/cm]   68
45.5432              75.7078
133.3548             165.2200             184.7946
259.9644             366.5061             398.6905
414.4397             511.2653             567.9423
574.8884             670.7863             708.0335
726.5467             781.3462             790.5871
809.7725             833.1259             857.6574
902.2324             919.0518             947.5098
951.2197             973.7752             976.7628
993.5417             1028.4880            1044.6899
1066.3727            1080.7651            1122.4186
1130.6728            1158.9654            1190.5294
1200.1796            1219.1873            1270.4320
1285.0749            1291.7671            1296.4883
1322.5729            1338.3505            1346.1564
1356.6654            1372.8200            1459.6888
1479.9061            1488.2148            1494.5896
1499.9868            1549.6878            1680.7271
2984.2936            3000.0566            3000.8528
3009.8591            3010.6797            3027.2708
3044.3417            3049.2270            3049.4701
3099.1227            3104.1923            3155.9040
3165.8517            3190.6002            3192.9221
ZeroEnergy[kcal/mol]   46.61
ElectronicLevels[1/cm] 1
0  2
End
!-----
!-----c10h15_R1-2_ts4-----

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Barrier      R1-2_ts4  R1-2_i3  R1-2_p1
RRHO
Geometry[angstrom]  25
C  -3.7925878631  1.1905256546  0.2266277512
C  -3.2515462295  1.9475431648  1.1792425901
C  -1.743011039  1.8490540823  1.1906173049
C  -1.4719611695  0.5851104159  0.3340700872
C  -2.7429090277  0.4453627896  -0.5626683625
C  -0.178068945  0.5088395564  -0.4201347757
C  3.2585214344  -1.0643405619  0.3540130182
C  3.5464685325  0.2686106655  0.1850501932
C  2.0934199016  1.2182254437  -1.0768551223
C  0.8589675452  1.3767187875  -0.3645301603
H  -4.8512512206  1.1358067776  -8.657024E-4
H  -3.8029303475  2.6028579713  1.8440249229
H  -1.3185603197  1.7689292276  2.1960095354
H  -1.3083902906  2.7490985007  0.7357526812
H  -1.5034893517  -0.2715878289  1.0232863833
H  -2.5888360869  0.9162741971  -1.542822019
H  -3.0006946122  -0.601395429  -0.7527374702
H  -0.0776601877  -0.3585149711  -1.0726817364
H  3.6059761494  -1.8099866273  -0.3523593534
H  2.5850021898  -1.4037266745  1.1321414633
H  4.358100524  0.5505991393  -0.4780055239
H  3.3649838589  0.9583752094  1.0019330248
H  2.1204259535  0.5016460053  -1.8904399082
H  2.699841372  2.103410747  -1.2379343984
H  0.7867232296  2.2367937569  0.2974725771
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  590.461
WellDepth[kcal/mol]  22.22
WellDepth[kcal/mol]  14.58
End
Frequencies[1/cm]  68
35.7815          49.2086
73.5434          96.8907          132.0561
189.7127        260.4861          282.2291
355.6388        386.0196          404.3172
446.2756        505.6610          653.1114
706.8729        727.8194          778.0437
789.1128        805.0893          812.4996
846.6948        850.2402          916.1537
945.7092        972.0713          973.3446
975.9256        987.2206        1011.4885
1025.1308       1035.0837        1053.2360
1124.1428       1134.2148        1156.8003
1170.8477       1213.2191        1242.1149
1264.8772       1288.9854        1291.8415
1310.9898       1324.6704        1336.0516

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1358.2129	1378.1783	1463.4163
1485.0958	1487.5121	1494.9835
1546.5305	1618.0240	1680.0394
2969.8673	2998.9879	3001.3637
3048.4481	3053.3698	3106.8301
3114.2864	3120.2692	3133.5754
3134.2602	3166.7478	3190.8461
3191.4342	3205.9540	3225.1082

ZeroEnergy[kcal/mol] 51.86

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R1_ts3-----

Barrier R1_ts3 R1 R1-3

RRHO

Geometry[angstrom] 25

C	-0.8126716586	0.3256390843	2.2841133076
C	-0.2188409406	-1.065489464	2.2873645625
C	0.7843634412	-1.0545315612	1.0999714885
C	-0.6082632743	1.0269870576	1.1096484438
C	1.4960102867	0.2752643012	1.1716000682
H	-0.9924294523	0.8435556406	3.2199226059
H	-0.9528632212	-1.8733705512	2.1735428364
H	0.298459474	-1.244886573	3.2365273298
H	1.4598598034	-1.9183945584	1.1427422337
H	-0.7416468406	2.1071621764	1.1074036261
H	2.0630877493	0.6236704364	0.3146738052
H	1.8894249772	0.5974123352	2.1307846042
C	-0.0327227113	-1.0527558932	-0.2074078544
C	-0.7880994706	0.3229178192	-0.2271316125
C	0.7776441373	-1.1071937489	-1.5267399304
C	-0.2736939482	1.0718943913	-1.4751007239
C	0.1293895649	-0.0523887597	-2.4429642185
H	-0.7465908576	-1.8814575417	-0.1843517279
H	-1.8616837085	0.1398202645	-0.3559904261
H	0.7766611146	-2.1071175776	-1.9676010564
H	1.8243752093	-0.8436652221	-1.3436012872
H	0.6023059621	1.6753201015	-1.2164000645
H	-1.0229426757	1.7486313861	-1.8946211967
H	-0.7650218338	-0.4698964923	-2.9194773152
H	0.7936708733	0.2855859489	-3.2426294983

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 560.623

WellDepth[kcal/mol] 29.16

WellDepth[kcal/mol] 19.6

End

Frequencies[1/cm] 68

133.5702	180.3828
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302.8861	317.6930	344.6354
386.7131	449.7555	514.8699
548.1907	580.7924	628.3337
664.8381	685.1329	767.2084
786.8740	793.7183	860.6026
867.3664	898.6219	905.3295
918.6362	928.3296	957.5581
968.4869	997.3383	1024.5574
1031.1847	1045.0637	1063.4430
1071.0583	1085.4903	1160.4773
1163.2495	1176.3309	1197.0736
1221.6640	1237.3798	1261.9435
1297.2286	1308.8591	1316.2394
1321.9714	1328.2508	1343.2139
1355.7794	1364.1549	1383.3714
1462.5716	1466.5317	1494.3181
1498.2668	1498.7614	1516.4865
3000.6182	3003.1912	3009.5212
3019.5002	3031.8313	3032.6031
3037.1204	3040.2977	3070.4035
3074.1206	3082.7677	3115.4968
3125.4190	3165.2971	3202.3346

ZeroEnergy[kcal/mol] 29.16

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R1-3_ts6-----

Barrier R1-3_ts6 R1-3 R1-3_i4

RRHO

Geometry[angstrom] 25

C	-1.6265498536	0.9053964481	0.9431961797
C	-1.6312875397	-0.5281199152	1.1280998112
C	-0.9566088502	-1.2586267359	-0.8485607968
C	0.3945677826	-0.5528358541	-0.8302941571
C	0.4085533135	1.0010579167	-0.5916696372
C	-0.7153395279	1.5831165576	0.221117205
C	-1.9347527208	-0.9587186082	-1.7601830144
C	1.4260825762	-1.1525736986	0.1791432183
C	1.7993714115	1.2347123131	0.0601401206
C	1.9756286773	0.0336190112	0.9966012925
H	-2.4747894098	1.4624639669	1.3394205487
H	-2.5783154825	-1.0077334942	1.354892048
H	-0.7752789998	-1.0137760924	1.5782183349
H	-0.9452999929	-2.2739977832	-0.459961238
H	0.8105154821	-0.6891049092	-1.8345138103
H	0.3846487969	1.5159475614	-1.5595944486
H	-0.8262256698	2.6618909478	0.1381624014
H	-1.9387232333	-0.021040298	-2.3047949189
H	-2.7977871361	-1.602132492	-1.8849540236
H	2.2358301073	-1.6406125186	-0.3704688226
H	0.9813629345	-1.9219045415	0.8153725178

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H  1.8661224447    2.1990175038    0.5692086562
H  2.5714782926    1.2173448822   -0.7181110439
H  3.0114307986   -0.1124103099    1.3126224628
H  1.3777937984    0.1853281422    1.9006951143
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  568.8602
WellDepth[kcal/mol]  29.64
WellDepth[kcal/mol]  22.71
End
Frequencies[1/cm]  68
81.7462          128.1152
179.4519          240.0178          247.6958
299.7790          374.7732          397.8876
456.9625          481.8008          548.0288
589.2027          600.1025          633.0419
697.0751          736.5187          776.0300
800.2452          836.9032          856.7076
868.5580          909.1142          931.2537
956.9074          972.2278          978.6620
997.7462          1018.3942         1034.4760
1054.1413         1070.8819         1114.2153
1158.9515         1166.5358         1182.6576
1237.8591         1256.9711         1272.6281
1277.3462         1289.1623         1317.3206
1329.9420         1341.2229         1352.7925
1376.9560         1418.8317         1423.7547
1484.2355         1495.2957         1497.6682
1516.8381         1534.6653         1642.3373
3000.6684         3012.5719         3022.9295
3034.7642         3041.0504         3067.6403
3077.9329         3086.0308         3099.7917
3122.3277         3129.6976         3132.3540
3137.2851         3213.0508         3218.8194
ZeroEnergy[kcal/mol]  39.20
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-3_ts10-----
Barrier      R1-3_ts10  R1-3_i4  R1-3_i6
RRHO
Geometry[angstrom]  25
C  -1.8494494714    1.6865487491    0.1876304179
C  -1.9903668494    1.86850824    -1.1469073452
C  -0.6891528563    1.2192884209    0.8902690933
C  -0.7360727898   -1.9768120661    0.2969269624
C  0.3054895698   -1.2915645014   -0.4139163858
C  0.5064060096    0.8067237143    0.3244414031
C  -2.0344307628   -2.0161787133   -0.0662936431

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C	1.7524432625	-1.5825732397	-0.0974702647
C	1.7577743212	0.5732267318	1.1551195352
C	2.1230445312	-0.9233119867	1.2383409075
H	-2.7066583632	1.9224458702	0.8141768008
H	-2.9204462836	2.2349141153	-1.5635104799
H	-1.1904610156	1.6661250076	-1.8503013103
H	-0.7936137502	1.1174726888	1.9680122305
H	-0.4497547411	-2.4771445552	1.2215498443
H	0.0611487336	-0.9977739037	-1.4303483501
H	0.6853453797	1.0945543889	-0.7073228405
H	-2.3855193413	-1.5241916228	-0.9668416584
H	-2.7724256006	-2.5404006694	0.5289301738
H	2.3945201269	-1.1889724492	-0.8921801846
H	1.9325424548	-2.6643155709	-0.051145185
H	1.6251923811	0.9860583808	2.1592441122
H	2.5892936072	1.1215629922	0.6986920882
H	3.1802827809	-1.0669345236	1.4822806274
H	1.5454036667	-1.3919034979	2.042286451
Core RigidRotor			
SymmetryFactor 1.0			
End			
Tunneling Eckart			
ImaginaryFrequency[1/cm] 522.6409			
WellDepth[kcal/mol] 25.81			
WellDepth[kcal/mol] 11.71			
End			
Frequencies[1/cm] 68			
39.1632	71.5540		
94.8700	148.6160	185.1864	
191.0213	232.4704	310.4063	
316.8477	348.9117	412.7089	
518.4848	578.5054	601.1056	
618.3880	656.5257	747.7172	
818.9005	848.0637	859.5246	
862.7122	877.0191	889.7351	
928.3254	964.3086	980.0872	
992.3146	1006.1739	1013.3902	
1031.0896	1056.1904	1095.3365	
1112.4128	1152.2412	1201.7050	
1226.2903	1264.6549	1271.8284	
1301.4230	1314.8042	1333.4546	
1337.1032	1344.5551	1353.6947	
1372.0989	1448.1030	1467.1835	
1485.7215	1490.3402	1503.3939	
1515.1517	1604.8075	1616.6473	
3001.5322	3019.8176	3023.9071	
3048.1546	3058.9620	3072.6682	
3110.0988	3121.7970	3133.4233	
3137.1800	3139.3172	3144.0630	
3148.4856	3223.4868	3223.8817	
ZeroEnergy[kcal/mol] 42.30			
ElectronicLevels[1/cm] 1			

```

0 2
End
!-----
!-----c10h15_R1-3_ts14-----
Barrier      R1-3_ts14  R1-3_i6  R1-3_p2
RRHO
Geometry[angstrom]  25
C  -0.6768814583   2.4265562626   2.208367187
C  -1.8085521445   1.7248820177   2.1003299345
C   0.6485027198   2.0192676074   1.7256646292
C  -1.0270565649  -2.0120427943  -1.1561190292
C   0.0566387372  -1.2982113472  -1.7848063478
C   0.8928471314   1.2357155853   0.6694348823
C  -2.3215556569  -1.6528148768  -1.2151451538
C   1.3677819926  -1.6582479459  -1.6909115765
C   2.2626413629   0.8142570683   0.2156634647
C   2.4712516582  -0.6732889398   0.2120129245
H  -0.7125859176   3.3878942754   2.7177518892
H  -2.7486844803   2.1166796149   2.4708556175
H  -1.8314963552   0.7387450369   1.6484786157
H   1.4966846458   2.4227226302   2.2778157742
H  -0.7561501272  -2.9090606227  -0.6015831606
H  -0.2050949526  -0.3986900513  -2.3379151061
H   0.0590702751   0.8621366419   0.0808662811
H  -2.6390882969  -0.7677352686  -1.7573468531
H  -3.0955633761  -2.23586854   -0.7314107726
H   2.1178870924  -1.1671051729  -2.2969667837
H   1.6451060888  -2.6150167024  -1.2632623513
H   3.0180014524   1.2912656579   0.8613956082
H   2.456079875    1.2062751523  -0.7939860734
H   3.4366381104  -1.0445853015  -0.1181250671
H   1.9792971888  -1.2610089872   0.9792444673
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  347.6853
WellDepth[kcal/mol]  34.9
WellDepth[kcal/mol]  5.26
End
Frequencies[1/cm]  68
18.7867          30.3379
59.9053          74.7135          112.5065
136.4203         165.9096          184.3548
245.1389         270.5595          307.4861
349.0387         408.7366          491.3133
525.3083         596.4694          604.6028
650.2559         726.6912          786.2654
828.8075         868.3025          890.6613
902.0339         908.1788          939.1560
952.7208         961.1085         1000.0073
1010.1431        1015.3484         1031.3396

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1041.3241          1061.0519          1092.8985
1119.4762          1200.9503          1226.1747
1281.5095          1307.2155          1314.8141
1318.9506          1349.7530          1360.5419
1394.6546          1451.9687          1456.3662
1460.8499          1469.5282          1565.2138
1633.9969          1677.5703          1708.6191
2948.2959          2980.2515          3108.3538
3112.4277          3119.6805          3124.8551
3133.0423          3133.9734          3135.5609
3138.5139          3150.2613          3211.0622
3217.5721          3221.7627          3228.0180
ZeroEnergy[kcal/mol] 65.49
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-3_ts7-----
Barrier          R1-3_ts7  R1-3  R1-3_i5
RRHO
Geometry[angstrom] 25
C -1.5455557684    0.79628938    1.1318012194
C -1.8086772997    -0.6361623741    0.7186792616
C -1.1011310666    -0.9535595501    -0.577997951
C 0.3099336709     -0.44019035     -0.698203689
C 0.3636802924     1.1050586037    -0.4877037277
C -0.5900849744     1.5545555014    0.5936920692
C -1.9204702644     -1.0759224226    -1.8279345545
C 1.335968916      -1.0168046944    0.3265522611
C 1.8372030357      1.3492442619    -0.1021558016
C 2.1808534474      0.1794227068    0.8394977952
H -2.1721797513     1.2026754852     1.9222911291
H -2.8868809601     -0.8003215031     0.6171919149
H -1.4862608283     -1.3008057842     1.5336037942
H -1.3946867367     -2.0748116671     -1.1709885752
H 0.6763517913      -0.6483846718     -1.7087104414
H 0.1157387371      1.6318577225     -1.4170622644
H -0.4657445334      2.5766314879     0.9467150597
H -1.4479414896      -0.9089928603     -2.7873504875
H -3.0002233097      -1.0442783132     -1.7623206851
H 1.9595516954      -1.7726727742     -0.1573033682
H 0.8267296706      -1.5179986618     1.1522712766
H 2.0006361663      2.3292086161     0.3555884757
H 2.4564159813      1.3041116059     -1.004899867
H 3.2514043753      -0.0376698309     0.85541224
H 1.8901682029      0.4317170865     1.8626139159
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 1935.5133
WellDepth[kcal/mol] 38.0

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WellDepth[kcal/mol]  43.26
End
Frequencies[1/cm]   68
56.7723              103.6407
146.9768              215.8505              296.3649
310.4519              362.3358              430.9991
458.5820              480.5418              547.6013
609.8074              636.9331              689.7876
708.4485              788.6213              805.2432
837.0550              848.0197              897.9023
903.0966              922.6822              953.3431
966.5058              979.6531              1000.9569
1004.3322             1032.0529              1057.8916
1100.5737             1153.0523              1162.6524
1183.3882             1190.6371              1199.5483
1246.2692             1253.5169              1271.5930
1292.3207             1310.7061              1314.8930
1327.9840             1334.1755              1346.6689
1359.4849             1392.9551              1415.5045
1421.4362             1480.5620              1490.3481
1495.7087             1514.2193              1707.2641
2173.1436             2977.3034              3008.5787
3021.6349             3030.7266              3037.2759
3040.2933             3050.6647              3064.7571
3073.6828             3093.6802              3115.1384
3130.3744             3140.8690              3246.0862
ZeroEnergy[kcal/mol]  47.56
ElectronicLevels[1/cm] 1
0  2
End
!-----
!-----c10h15_R1-3_ts11-----
Barrier      R1-3_ts11  R1-3_i5  R1-3_i7
RRHO
Geometry[angstrom]   25
C  -1.9225008068    1.5272745387    1.1441923316
C  -2.389731452    0.2394572372    0.5239050407
C  -1.3854920078   -0.4597567587   -0.3631713996
C   0.0334734604    0.0289359341   -0.395290935
C   0.4037942823    1.3655376464    0.2359025329
C  -0.6875516433    2.0152181983    1.0348081176
C  -1.6699164996   -1.8957850482   -0.7094643753
C   1.2532511831   -0.8838311732   -0.4264219171
C   1.6982054996    1.0219520722    1.0135167171
C   2.4015780514    0.0113760846    0.0936754997
H  -2.6613301166    2.0711056801    1.7271611717
H  -3.3354660904    0.4079885151   -0.0105722923
H  -2.6582432781   -0.4529900918    1.3423171578
H  -0.8217487511    0.1726044196   -1.3692683001
H   0.6993267509    2.0807707278   -0.550502623
H  -0.4396606136    2.9567058572    1.5195270056
H  -1.5309095638   -2.5585079646    0.1596595876

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H  -1.0162268935   -2.2658160697   -1.5035580869
H  -2.7042536011   -2.0237795519   -1.0449516454
H   1.4762165479   -1.3011676731   -1.4133522443
H   1.1044443504   -1.7392294841    0.2471334859
H   1.4346545369    0.548467454    1.9658297984
H   2.3066011308    1.9036049726    1.2342703947
H   2.8729750486    0.5408222184   -0.7412170572
H   3.1830144754   -0.5597007409    0.600386035
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 1989.9191
WellDepth[kcal/mol] 41.83
WellDepth[kcal/mol] 42.07
End
Frequencies[1/cm] 68
74.9625          99.1617
187.6763         207.7134         237.4188
266.9293         325.1129         410.4889
430.9467         435.0413         503.4889
541.5019         559.1585         664.3753
718.9398         785.6171         844.9680
880.8749         899.7889         914.8697
921.3475         936.5062         992.9898
1000.6505        1016.8825        1030.2294
1046.9309        1057.1563        1094.1391
1123.5428        1139.2794        1184.4951
1194.9896        1210.5253        1229.9306
1235.3112        1264.2295        1303.6528
1307.9500        1318.0227        1337.6836
1350.1140        1360.9602        1381.7462
1416.9865        1418.6989        1468.8376
1482.5656        1490.3885        1490.4490
1499.3639        1508.1591        1715.8813
2143.0565        2915.1634        2921.8070
2949.9481        2982.9754        2985.5023
3021.9257        3024.7265        3036.3843
3040.7600        3070.0185        3082.3425
3084.2593        3124.4672        3148.5683
ZeroEnergy[kcal/mol] 46.13
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-3_ts15-----
Barrier      R1-3_ts15  R1-3_i7  R1-3_p4
RRHO
Geometry[angstrom] 25
C  -1.9872052078    0.9190431572    0.9996975389
C  -2.3889412036    0.1904960444   -0.260100592
C  -1.2373327939   -0.5997927531   -0.8516387223

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C	0.0405598807	-0.1604029821	-0.6761900124
C	0.3991811192	0.9110685543	0.3296658329
C	-0.7213537478	1.2254153568	1.2811301497
C	-1.4163005038	-2.4983867271	0.4498054794
C	1.3098538466	-0.8077534484	-1.1852530699
C	1.7347852373	0.3964397479	0.9113133599
C	2.4454058159	-0.1829767975	-0.3291878711
H	-2.7799590766	1.1984942496	1.6878383752
H	-2.7582982508	0.9177403634	-1.0003430499
H	-3.2379374614	-0.4686191281	-0.0549687823
H	-1.4664134028	-1.2634794065	-1.679010785
H	0.6384641513	1.8382962301	-0.2234994067
H	-0.4754818653	1.7572380424	2.1967111972
H	-1.4217223734	-2.0538482908	1.4369068374
H	-0.5353518542	-3.0681565992	0.1797674965
H	-2.3626618483	-2.879914417	0.0828682739
H	1.4690673149	-0.640869819	-2.2563165649
H	1.2600814244	-1.8937273943	-1.0466402596
H	1.5333576089	-0.3935749158	1.6429511755
H	2.3161801151	1.176025989	1.4107772185
H	2.9283357999	0.6285409734	-0.8828836798
H	3.2240682757	-0.9044130297	-0.0732791391
Core RigidRotor			
SymmetryFactor 1.0			
End			
Tunneling Eckart			
ImaginaryFrequency[1/cm] 458.4129			
WellDepth[kcal/mol] 30.83			
WellDepth[kcal/mol] 8.6			
End			
Frequencies[1/cm] 68			
60.5539	104.1306		
115.8269	154.9892		180.2193
243.8827	306.0208		365.7366
434.3474	487.4014		498.4056
514.4224	543.3242		565.1646
615.0370	699.5374		749.5652
802.2790	814.3940		849.8770
883.6556	897.2594		905.5670
915.0415	961.7895		985.5203
997.1822	1008.5333		1027.6479
1069.4825	1086.6159		1126.5962
1161.6446	1191.2902		1194.3043
1212.3210	1233.6246		1278.4058
1297.3043	1300.8575		1324.4398
1336.6997	1358.0277		1372.3782
1412.8822	1420.7975		1426.2825
1476.4253	1479.6539		1495.4929
1510.2416	1572.9526		1709.0937
2902.4188	2963.9779		3012.9982
3026.4225	3028.6905		3041.8355
3045.5917	3074.8844		3080.6228

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3087.7014          3132.3039          3148.3762
3156.5652          3229.8597          3243.6977
ZeroEnergy[kcal/mol] 34.89
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-3_ts1-----
Barrier          R1-3_ts1  R1-3  R1-3_i1
RRHO
Geometry[angstrom] 25
C -1.7874943823    0.5976260084    1.3112770767
C -1.8814897041    -0.9124144551    1.3410927596
C -1.6892934625    -1.5890998308    -0.0054916304
C 0.3654989597     -0.6744073667     -0.422904967
C 0.2684756945     0.8265009265     -0.2067431768
C -0.8874823259     1.3166003785     0.6419017603
C -2.4742007908     -1.30844736     -1.0825679999
C 1.3845160106     -1.2690596901     0.533265457
C 1.6149142618     1.1457721662     0.5169999841
C 1.8445379462     -0.0826634092     1.4126475922
H -2.5210717229     1.1342868967     1.9071546838
H -2.8605429698     -1.1985930196     1.7415795145
H -1.1504857494     -1.3127519671     2.0537580997
H -1.1860129509     -2.5514695791     0.0172607158
H 0.3651901327     -1.0323674125     -1.4449001551
H 0.2198918509     1.3561995936     -1.1651171094
H -0.9401041477     2.4007433243     0.7278781219
H -2.4309719307     -1.9137854646     -1.9806302201
H -3.1026069304     -0.4251590653     -1.1120818142
H 2.2306098485     -1.6820249393     -0.0313698257
H 0.9895402405     -2.0999368504     1.13098042
H 1.5846296501     2.0869600532     1.0723455005
H 2.4155649465     1.2227624435     -0.2265689841
H 2.8806932192     -0.1793729147     1.7447485481
H 1.2191763062     -0.0077254664     2.3070566484
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 403.5346
WellDepth[kcal/mol] 30.35
WellDepth[kcal/mol] 9.8
End
Frequencies[1/cm] 68
54.4655            115.4470
155.6252            192.5474            246.3443
290.1468            325.3689            395.3143
453.2055            514.5458            533.8350
590.8433            693.9154            708.1334
760.5387            793.2367            817.7801
829.0790            843.7545            860.3652

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890.3580	898.9488	931.1522
949.9969	961.8762	985.5938
1003.6314	1005.4769	1018.5669
1038.6930	1093.9829	1111.3133
1155.0182	1174.9486	1214.1191
1235.8198	1243.2481	1263.0549
1290.3223	1299.6863	1311.9862
1342.9839	1346.3099	1349.2611
1357.6771	1408.2506	1431.4929
1476.1005	1491.1971	1493.2968
1506.5890	1556.9453	1714.8354
2994.7638	3010.3505	3011.7156
3013.0566	3028.7064	3031.4358
3042.0074	3072.8821	3086.9626
3112.8559	3129.4585	3136.8098
3143.8529	3171.8494	3217.6188

ZeroEnergy[kcal/mol] 39.91

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R1-3_ts2-----

Barrier R1-3_ts2 R1-3_i1 R1-3_p6

RRHO

Geometry[angstrom] 25

C	-1.5682616797	0.0913930266	1.1182766931
C	-2.0471280622	-1.1170594577	0.3531256604
C	-3.2300747864	-0.8755221308	-0.5560782245
C	1.8420768257	-0.9608055494	-0.1856576881
C	1.1912363414	0.1265389319	-0.6722143305
C	-0.4122515419	0.7028548864	0.9797357616
C	-3.7325853145	0.3071977447	-0.8971231873
C	3.1566296167	-0.5962227972	0.4543791476
C	2.077543279	1.3545789699	-0.581718035
C	3.1171019262	0.9534541962	0.4918802953
H	-2.2817791267	0.4793576262	1.8552264938
H	-2.3242197783	-1.9022742879	1.0702840345
H	-1.2235230074	-1.5364204484	-0.2347457627
H	-3.6861982871	-1.7775627687	-0.9607855407
H	1.4773980899	-1.9795203394	-0.2444543043
H	0.3402589297	0.0804749228	-1.33902592
H	-0.0059346527	1.5546619234	1.5122900208
H	-4.5830212343	0.3840858425	-1.5651330969
H	-3.3101237544	1.235380404	-0.52784276
H	3.9927575741	-0.9636739933	-0.1579092006
H	3.2896941077	-1.0383230701	1.4477896475
H	1.5357662404	2.2694415086	-0.3307418892
H	2.5572140039	1.5279507297	-1.5541264333
H	4.0959703827	1.4070186128	0.3245693389
H	2.7689029083	1.2817175174	1.4751072795

Core RigidRotor

SymmetryFactor 1.0

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End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  315.5733
WellDepth[kcal/mol]  35.38
WellDepth[kcal/mol]  3.11
End
Frequencies[1/cm]  68
11.1885          30.2188
77.0384          81.7684          120.1806
164.0627        173.9558          224.0339
282.2271        377.5260          453.3460
513.9089        577.0999          611.2848
685.3959        722.7374          775.2804
827.0954        846.8842          875.5646
882.2324        903.6323          908.9691
919.0300        929.3669          941.6017
953.0653        967.5309        1030.7535
1034.3773       1052.9826        1061.0185
1109.9676       1117.9209        1139.8573
1213.5465       1216.5089        1231.2836
1277.8191       1307.7139        1317.2862
1322.7209       1325.6946        1348.4960
1375.1541       1443.6432        1471.6794
1478.6256       1489.3358        1505.7209
1544.1069       1669.3401        1704.3622
2982.6272       2995.5388        3001.8264
3013.6538       3029.3622        3045.5982
3046.3034       3070.3941        3090.8924
3118.4379       3136.4056        3178.0447
3185.4286       3200.6233        3215.8155
ZeroEnergy[kcal/mol]  65.49
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-3_ts4-----
Barrier      R1-3_ts4  R1-3_i1  R1-3_i2
RRHO
Geometry[angstrom]  25
C  -1.2159492486    0.4901838926    0.4259163675
C  -1.3598119683   -0.9937904059    0.2578507861
C  -2.7701902726   -1.4746056314    0.0089150314
C   1.4753139174   -0.2365134456   -1.1661241675
C   0.7801816045    0.9571711339   -1.070487721
C  -0.3089494224    1.3030637677   -0.1355508275
C  -3.8110551291   -0.7284110478   -0.3491294362
C   2.0506559759   -0.860307755    0.0804712015
C   2.4030593032    1.6137308425    0.3838134633
C   2.3291051539    0.2950397395    1.1025443586
H  -1.962920012    0.9544319928    1.0663430611
H  -0.9826904796   -1.5049099476    1.1573024608
H  -0.7175918537   -1.343480344    -0.5593546375

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H -2.9117102236 -2.5478998716 0.1228269498
H 1.9698501689 -0.4566179116 -2.1073937917
H 0.7816055685 1.5883216029 -1.9605045571
H -0.4163984743 2.3672475222 0.0609832639
H -4.7856568644 -1.1709507545 -0.5212345734
H -3.7286141142 0.3435499696 -0.4926914376
H 2.9807020031 -1.3733674334 -0.1820785902
H 1.4094961314 -1.6190915215 0.5424523118
H 2.0498008509 2.5088993855 0.8848833212
H 3.2271284607 1.7731253109 -0.3051566819
H 3.2551749615 0.0836525991 1.6515994302
H 1.5288849627 0.3341363109 1.8449784143
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 540.0079
WellDepth[kcal/mol] 33.7
WellDepth[kcal/mol] 21.27
End
Frequencies[1/cm] 68
38.2614 66.8384
112.7030 132.8080 157.3244
169.8789 230.7889 275.2897
371.3192 414.0919 507.1369
532.4685 560.0374 594.8725
619.2407 666.6122 732.7793
775.7193 784.3788 831.7198
861.3303 866.9861 918.7476
933.9262 935.5973 941.1844
957.3561 1004.3567 1016.1094
1034.0001 1042.8791 1055.5227
1100.1206 1109.9605 1192.7194
1218.3046 1223.8795 1226.5473
1281.6834 1323.9002 1328.7680
1338.3854 1345.4078 1400.9295
1436.0444 1450.6563 1460.5169
1465.6575 1475.4380 1490.9503
1507.4025 1685.6224 1704.6154
2968.6016 3006.9365 3019.2142
3024.8205 3049.1876 3074.5126
3089.3497 3112.7662 3117.9334
3120.8371 3136.1886 3140.9332
3149.1774 3204.1002 3214.2431
ZeroEnergy[kcal/mol] 63.81
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-3_ts8-----
Barrier R1-3_ts8 R1-3_i2 R1-3_p1
RRHO

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```

Geometry[angstrom]    25
C   -1.7347733916      0.5973188068      0.2871769537
C   -1.7340421018      -0.866673978      -0.0422391189
C   -3.0716867749      -1.4177119506      -0.4811879314
C    1.2687891511      0.5624178605      -1.0548912573
C    0.2033303371      1.4085099897      -1.1296213923
C   -0.9164790537      1.545917965      -0.1964072673
C   -4.1394484406      -0.7127245885      -0.8428024386
C    1.6202315288      -0.3081071174      0.0260871937
C    4.2730138322      0.770846024      0.6879654241
C    3.0213366658      0.7024836729      1.2587514595
H   -2.5239760782      0.9171153902      0.9639409564
H   -1.4083479907      -1.4410345426      0.8383408958
H   -0.990345253      -1.0813248204      -0.816905853
H   -3.1280796885      -2.5044210803      -0.5084816395
H    1.9884483431      0.6195566937      -1.8689365881
H    0.196647648      2.1169510664      -1.9561232188
H   -1.144361181      2.5737901442      0.0867587026
H   -5.0542530792      -1.2022564845      -1.1570946424
H   -4.1381488533      0.3719177442      -0.8482161835
H    2.2482645284      -1.1619556005      -0.1966935627
H    0.8932025851      -0.4740070819      0.8118577012
H    4.5445223544      1.5757784362      0.0147303928
H    4.9933074916      -0.030265265      0.8095040468
H    2.8612687178      0.0020039731      2.0725745097
H    2.4071877033      1.5949977428      1.2987118574
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm]  621.9447
WellDepth[kcal/mol]  24.38
WellDepth[kcal/mol]  19.6
End
Frequencies[1/cm]  68
38.4460              44.4016
62.7924              66.0576              118.8537
149.6620            156.9524              206.5123
254.8443            296.3638              379.1912
408.1921            443.4844              518.8681
543.4434            606.0133              690.0873
746.9874            775.9163              790.7887
808.8814            816.7500              836.8571
874.3171            933.9172              941.0500
956.6102            986.0147            1008.2203
1013.0066           1022.3861            1037.3780
1045.8652           1067.5135            1111.3060
1143.1113           1229.3042            1242.5467
1250.5453           1268.8172            1284.9761
1329.8057           1342.9110            1417.0577
1442.6705           1454.3408            1463.9551
1465.5551           1495.3250            1540.1512

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1581.1435          1679.0541          1705.7167
2975.8864          3047.0167          3094.9973
3113.0234          3114.3850          3121.6422
3132.4339          3133.4328          3135.6783
3138.3050          3139.3616          3192.8623
3214.9069          3224.4059          3225.2981
ZeroEnergy[kcal/mol] 66.92
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-3_ts5-----
Barrier      R1-3_ts5  R1-3_i1  R1-3_i3
RRHO
Geometry[angstrom] 25
C -1.5655072614    1.1559493028    0.1380742397
C -1.7795760991    -0.0696842934    0.9844518232
C -2.7181652885    -1.0997773422    0.3962365748
C 0.9986932859     -0.5321064309    -0.9029612086
C 0.9146644998     0.91799732     -0.5022985897
C -0.451836827     1.5652721088    -0.4762848052
C -3.1699915895    -1.1291908912    -0.8541010217
C 2.2680642043     -1.033111932     -1.0304553914
C 1.6826367805     0.9697891919     0.8836941728
C 2.8807729817     0.0542651707     0.8505654792
H -2.4516867687     1.7767271545     0.0202209943
H -2.1931557743     0.244511913      1.9534206106
H -0.8311301997     -0.5612695869     1.2233663173
H -3.0256306807     -1.8835589618     1.0863946565
H 0.1509720786     -1.1874337085     -0.7381777456
H 1.5316248084     1.4905754974     -1.2059646216
H -0.5228028855     2.5006624198     -1.0266073731
H -3.8360613471     -1.915231878     -1.1914892173
H -2.8881965638     -0.3753768914     -1.5813284978
H 3.0548388133     -0.4314546041     -1.4728052292
H 2.4462899287     -2.1037281469     -1.0541420762
H 0.9923111147     0.6647029175     1.6729143618
H 1.9696234376     2.0048362937     1.0972548063
H 3.833746054      0.4612386905     0.5281144769
H 2.9554772978     -0.7369053132     1.5871282637
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 569.2417
WellDepth[kcal/mol] 34.42
WellDepth[kcal/mol] 16.73
End
Frequencies[1/cm] 68
44.0803          67.5156
95.6382          146.0509          154.7044
188.1686         272.7644          272.9665

```

390.3966	441.7793	460.1159
495.0563	543.0527	559.6824
605.7071	674.6012	707.7764
734.6390	773.2335	816.0544
842.1312	889.5457	901.7720
927.8156	938.8605	946.6185
954.2712	1013.7514	1014.9027
1032.2242	1036.5484	1045.4367
1060.2171	1103.9181	1146.1893
1221.8207	1237.4610	1262.5742
1273.6223	1302.0526	1318.2316
1327.1934	1341.7908	1349.6291
1431.8093	1434.5972	1448.0266
1464.3536	1476.6640	1492.7265
1547.6074	1702.7750	1714.3652
2991.0522	3000.5134	3031.1957
3048.5099	3084.1109	3114.5739
3117.3209	3119.8678	3122.9982
3136.4411	3139.4081	3172.8219
3196.5646	3214.1101	3216.3636

ZeroEnergy[kcal/mol] 64.53

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R1-3_ts9-----

Barrier R1-3_ts9 R1-3_i3 R1-3_p1

RRHO

Geometry[angstrom] 25

C	-1.565172054	1.0976606133	0.4268803019
C	-1.7550680857	-0.1599614265	1.2289014592
C	-2.5596182099	-1.2500146691	0.5537447426
C	1.0941830841	-0.452612189	-0.4964449873
C	0.8918438512	0.9780993329	-0.2653356281
C	-0.4519106928	1.558757764	-0.1766356341
C	-2.9267411324	-1.2785943589	-0.7238171966
C	2.2070577996	-0.9783502638	-1.0280954725
C	1.7180077925	1.4181005222	1.5641004422
C	3.0987327865	1.2810664895	1.53202459
H	-2.4567283109	1.7142809544	0.3400463623
H	-2.2732324997	0.1036621765	2.1616792955
H	-0.7949220212	-0.579337191	1.547754082
H	-2.8423961459	-2.0761477824	1.2039421767
H	0.2841982562	-1.12319951	-0.2288467609
H	1.5731480107	1.5963548563	-0.8417897762
H	-0.5389991568	2.5404420019	-0.6386635871
H	-3.5007457234	-2.1065966067	-1.1240420204
H	-2.6643646566	-0.4812772818	-1.4108157934
H	3.0447244086	-0.3561782285	-1.3274809248
H	2.3089964937	-2.0459127579	-1.1834222875
H	1.1395489313	0.6751813106	2.1027372925
H	1.3051469102	2.419824169	1.6209050275

```

H 3.7382994386 2.1057624189 1.2376602613
H 3.5732389264 0.3168376561 1.6686960351
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 641.8748
WellDepth[kcal/mol] 19.12
WellDepth[kcal/mol] 19.6
End
Frequencies[1/cm] 68
41.1369 55.5396
77.4544 104.8509 121.2363
136.5650 168.6195 242.2781
264.6901 281.9607 312.5874
420.6217 427.6980 445.6937
562.2125 599.1873 657.5125
720.5934 752.5396 775.3134
798.2427 853.6434 878.2225
907.8793 932.2850 950.6893
962.7968 991.4315 1001.0497
1014.3811 1022.8692 1038.6629
1066.6700 1077.5472 1104.6442
1188.1955 1224.8154 1234.0622
1246.3072 1301.0994 1323.3923
1329.7790 1341.4453 1365.9980
1435.2908 1448.0758 1461.6038
1464.7525 1483.9618 1530.7316
1636.4288 1653.9300 1702.5260
2992.9600 3043.5433 3110.8929
3115.7022 3119.6708 3129.4405
3134.3471 3135.4300 3136.9567
3145.1736 3167.3746 3190.8882
3216.9904 3217.0497 3228.1998
ZeroEnergy[kcal/mol] 66.92
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```

R1_secondary_c8h11

```
!-----c10h15_R1-2_rpl-----
Well          R1-2_rpl
Species
RRHO
Geometry[angstrom]  19
C  -2.7342652128    0.0868348208    0.1142223458
C  -2.17523837     0.8708570487    1.0339971935
C  -0.6657869164    0.7997156964    0.9967141277
C  -0.3998700166    -0.4732347302    0.1496030959
C  -1.6992090855    -0.6539149341    -0.6980813907
C  0.865589892     -0.5320380491    -0.6470782032
C  3.1171985769     0.2134977531    -1.2841406194
C  1.9523577186     0.3223051836    -0.5460238216
H  -3.7988001954    0.0092568819    -0.0759145497
H  -2.7157165273    1.5281096467    1.7057056102
H  -0.2084556906    0.7429052029    1.9891852271
H  -0.2611562631    1.6992271408    0.5138423326
H  -0.3915406177    -1.3192541392    0.8544631028
H  -1.5903897173    -0.1995306465    -1.6920421579
H  -1.9424543037    -1.7089934153    -0.8582067352
H  0.9422161521     -1.3611600609    -1.3493308294
H  3.2481342117     -0.5783721538    -2.013667951
H  3.9323757046     0.9142474078    -1.1580698877
H  1.8908876604     1.1410603461    0.1673451102
Core RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
63.8015           104.0616           158.9477
189.0436           357.5374           379.2804
404.2592           496.1074           547.1269
657.7944           705.9635           759.0884
778.8509           795.9983           831.2846
914.8626           943.9012           962.5313
972.7504           976.0345           994.9048
1027.8009          1046.1388          1124.2622
1132.4915          1156.3160          1199.5800
1213.1770          1281.8005          1286.6122
1293.8460          1307.6878          1339.3387
1356.6498          1374.4126          1487.9488
1494.9522          1499.4856          1522.2185
1679.8045          2953.3989          2998.6192
3000.0307          3049.4063          3053.4186
3115.2666          3135.9380          3138.1764
3167.5727          3192.0912          3232.8217
ZeroEnergy[kcal/mol]  37.28
ElectronicLevels[1/cm]  1
0  2
End
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End
!-----
!-----c10h15_R1-2_ip4-----
Well          R1-2_ip4
Species
RRHO
Geometry[angstrom]  19
C  -2.6193406386   1.6718406703   -0.2947172116
C  -1.9286087451   0.6869330424    0.400435497
C  -0.486636773    0.7439363829    0.8236983543
C   0.2370237189   -0.5439614746    0.5168359669
C  -2.1364291658   2.8920078343    -0.72714735
C   1.3246916042   -0.7125100915    -0.2505318739
C   3.1550469257   0.0670874597    -1.704129682
C   2.0647507707   0.3144554836    -0.9691876538
H  -3.6613628748   1.4522953588    -0.5180547754
H  -2.4706588085   -0.2137358548    0.6744710669
H  -0.4448983707   0.9083838467    1.9129583315
H   0.0171572873   1.5979154515    0.3709183403
H  -0.1950698471   -1.4297543436    0.9776881864
H  -1.1154654837   3.2084321247    -0.55242584
H  -2.7756668811   3.5799717096    -1.2652382577
H   1.7117230375   -1.7237092879    -0.3586862168
H   3.5558883814   -0.9370057588    -1.8028125073
H   3.6789486581   0.8569860169    -2.2287284967
H   1.7038192045   1.3368874297    -0.9042948784
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
12.3892           35.9172           126.6108
173.8492          214.9109           269.5503
314.7950          378.6613           429.1142
538.1800          569.7017           625.3861
667.0509          697.7251           787.3539
805.8499          900.3086           912.9120
932.2039          984.6525           994.3769
997.4592          1009.0177          1039.3880
1051.9372         1145.3891          1200.9368
1220.2403         1241.3078          1284.6219
1302.1286         1330.5891          1401.3892
1434.5644         1469.6419          1471.1413
1480.1934         1525.1162          1656.1633
1708.7514         2951.3917          3098.4374
3118.9792         3124.8594          3130.8450
3140.3929         3147.0592          3151.9282
3154.2415         3218.8864          3236.4663
ZeroEnergy[kcal/mol]  36.81
ElectronicLevels[1/cm]  1
0  2
End
End

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!-----
!-----c10h15_R1-1_ip7-----
Well      R1-1_ip7
Species
RRHO
Geometry[angstrom]  19
C  1.7267098468   -0.1193459889   0.2757292955
C  2.8805695999   -0.2958150049   -0.3604566957
C  -1.9067127043   -1.3430999331   -0.1650343985
C  -2.5267242332   -0.2300777801   -0.553380171
C  -0.4097983519    1.0718723365   -0.2270345876
C  0.361844015    -0.2081548855   -0.3550210554
C  -0.4539218974   -1.3913649406    0.2321851248
C  -1.8516267742    1.1158307366   -0.6136294818
H  1.733730748     0.1068888368   1.3415797267
H  3.8321457577   -0.2220455462    0.1541402768
H  2.9154020272   -0.5201650876   -1.422604171
H  -2.4622275847   -2.2760756531   -0.1189927972
H  -3.5762289876   -0.2648637405   -0.8323217593
H  0.1255187674    2.0027839705   -0.075419722
H  0.4978990283   -0.4284296335   -1.429240255
H  -0.0026574408   -2.3338778303   -0.0951372704
H  -0.3709774927   -1.3826810328    1.3277712734
H  -1.9680907209    1.530954393   -1.6326071897
H  -2.3933516025    1.8273147836    0.0269278575
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
85.9873           99.9079           134.4186
277.9510          303.2116           381.4284
406.1786          419.5016           523.3190
556.3728          667.0090           680.6167
767.4470          877.1487           902.7569
927.4041          946.9542           949.4813
965.7196          997.9338          1015.4984
1034.4299         1058.0230          1127.4247
1146.9227         1175.9960          1197.8708
1211.9908         1269.0295          1306.7365
1318.9915         1326.4165          1357.5522
1392.9390         1417.8386          1452.3851
1454.5076         1480.5519          1705.2871
1718.2393         2900.6317          2909.3953
2981.3626         2994.9335          3044.0997
3112.6736         3125.9605          3131.8843
3155.4755         3166.8898          3207.0472
ZeroEnergy[kcal/mol]  46.61
ElectronicLevels[1/cm]  1
0  2
End
End
!-----

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!-----c10h15_R1-1_ip3-----
Well          R1-1_ip3
Species
RRHO
Geometry[angstrom]  19
C   2.0069210336    1.2462451866    0.1465129964
C   2.0780616429    2.0666980102    1.1907424041
C   -0.8512401985    1.3044782128    -0.9946375095
C   -2.1541631237    1.1944692997    -0.9738532863
C   1.9632483622    -1.2103421392    -0.0105660516
C   1.1023390037    0.0369909243    0.0400443918
C   0.1223881389    0.1596614752    -1.1496104471
C   2.0591485532    -2.0859652981    -1.0071986596
H   2.651014671    1.4177030556   -0.7152057052
H   2.7605832265    2.9091912379    1.2060282145
H   1.4558437496    1.9248188537    2.0692884006
H   -0.4034457849    2.2988107091    -0.8827241478
H   -3.012767832    1.8430781826    -0.8822045912
H   2.573119216    -1.3599725291    0.8782735015
H   0.5065438745    -0.0143669569    0.9606664191
H   0.6978922599    0.3031392259    -2.0730583657
H   -0.4353535216    -0.7730066882    -1.2584237506
H   2.723045289    -2.9401354327    -0.9355561749
H   1.4871674395    -1.9960083293    -1.9235906385
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
74.5213           87.5766           100.2543
102.4510          192.9812           272.4975
312.7586          347.9478           385.1290
443.7223          564.4640           623.9156
668.0200          695.8510           786.0590
827.3156          853.9582           942.8407
948.8619          951.4391           966.5376
1000.2228         1034.3992          1039.8431
1062.4768         1131.4820          1143.0404
1225.9506         1261.5105          1291.6314
1318.4832         1320.9639          1338.0803
1360.5901         1447.6829          1451.7247
1486.4048         1676.4411          1691.5359
1703.6850         3001.5980          3014.2561
3022.9136         3082.8243          3115.7897
3125.1966         3127.9860          3141.3649
3208.9669         3216.8698          3236.4230
ZeroEnergy[kcal/mol]  77.92
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----h_c8h10_R1-2_p2-----

```

```

Bimolecular      R1-2_p2
Fragment          c8h10
RRHO
Geometry[angstrom]  18
C   2.3848724066    0.0851699942   -0.44696053
C   1.9496291815   -1.1134474851   -0.0634291954
C   0.5150680625   -1.0731506851    0.4076073617
C   0.2504279874    0.4421427011    0.5921174162
C   1.3197497372    1.1459791843   -0.3007082257
C   -1.1616310819    0.9196289995    0.340547217
C   -3.1849913003   -0.5296788451   -0.4418293405
C   -2.1695526561    0.1907972641   -0.0533478936
H   3.3662151666    0.290458995   -0.8596624225
H   2.5249755505   -2.0308166393   -0.1161773656
H   0.3453876507   -1.6348781025    1.3311529756
H   -0.152601353   -1.5076783408   -0.347289416
H   0.4986251337    0.6937852781    1.6308597056
H   0.9038043055    1.4146698449   -1.2806340105
H   1.68831543     2.0730887142    0.1500335773
H   -1.3400865284    1.9822725181    0.5058166868
H   -3.4086010576   -0.6741260158   -1.4949076218
H   -3.8461166349   -1.0107763798    0.2733160814
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  48
52.9651           101.1055           143.1641
295.8670          335.0526           376.0033
397.6293          508.9343           604.8305
682.6865          713.4168           781.1854
822.6738          873.5848           906.6469
919.8111          945.5932           974.0090
975.4189          992.4645          1022.1191
1038.7888         1081.0300          1129.1766
1156.0592         1161.2161          1204.7038
1290.8210         1295.5908          1317.4896
1350.3848         1359.8886          1380.1637
1478.6739         1488.7167          1496.3461
1680.7515         2050.2970          2997.6941
3004.4982         3011.6247          3047.4031
3055.4936         3102.3188          3110.5803
3167.0120         3180.6879          3191.6368
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment          H
Atom
Mass[amu]  1
ElectronicLevels[1/cm]  1
0  2
End

```

```

GroundEnergy[kcal/mol] 91.06
End
!-----h_c8h10_R1-2_p3-----
Bimolecular R1-2_p3
Fragment c8h10
RRHO
Geometry[angstrom] 18
C -2.8075270574 -0.0226640657 0.2301375134
C -2.241251968 0.8543803496 1.0558181908
C -0.7521275518 0.9747827937 0.8337697284
C -0.4872580226 -0.0061046874 -0.303438129
C -1.8059584735 -0.6574893993 -0.7034050135
C 0.6978604024 -0.2687965342 -0.8732101016
C 3.1370937712 0.064484604 -1.0896713706
C 1.9643475094 0.3415029288 -0.5060963122
H -3.8625851809 -0.2691749644 0.2108747592
H -2.7654264895 1.4295052608 1.8100807061
H -0.1832186839 0.7212690061 1.7380588624
H -0.4609210133 2.000144893 0.5701559639
H -2.0510334123 -0.4694504457 -1.757053701
H -1.7733438858 -1.7490136039 -0.5891947208
H 0.7355201304 -0.998316751 -1.6807876827
H 3.2117754434 -0.6562867153 -1.8981668067
H 4.0552415917 0.5481444156 -0.77887829
H 1.9440508905 1.0717509153 0.2994104037
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 48
61.4193 136.5623 149.4245
219.4409 373.1623 381.1176
431.4817 444.7285 675.6935
692.9344 694.2082 797.8069
819.4924 883.2869 922.9221
949.1506 950.5799 970.3380
980.1421 980.6638 999.2278
1032.6624 1114.4101 1131.3630
1161.8383 1185.6870 1217.1026
1291.2719 1294.1241 1325.1651
1342.5433 1380.2051 1456.3849
1467.3923 1473.5420 1661.8130
1685.4967 1718.7135 2994.2603
2997.2100 3010.3737 3011.9712
3117.1129 3130.1843 3139.6271
3174.3464 3198.3736 3218.0843
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1

```

```

ElectronicLevels[1/cm]      1
0    2
End
GroundEnergy[kcal/mol] 74.81
End
!-----c4h6_c4h5_R1-2_p5-----
Bimolecular      R1-2_p5
Fragment          c4h5
RRHO
Geometry[angstrom]      9
C  -1.4487222083    -0.4326185116    1.1031699213
C  -0.3744895678    -0.5882569411    0.3591530666
C  1.4230480216     0.2817445099    -1.0933344666
C  0.3337242867     0.4785109378    -0.345060996
H  -2.111970598     -1.0471459191    1.6924022963
H  0.0412467171     -1.5969553749    0.2444009964
H  1.8527839396     -0.7066696673    -1.2223110857
H  1.9181983615     1.1016381266    -1.5990951602
H  -0.0744509523     1.4789258396    -0.2334905721
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 21
178.7824          301.9654          513.7116
563.9794          727.3379          786.4375
862.8538          937.6451          948.6567
1031.1551         1174.8299         1252.5578
1317.1948         1443.7437         1631.3541
1684.1465         3015.4742         3133.3427
3153.5072         3221.8621         3247.0440
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]      1
0    2
End
Fragment          c4h6
RRHO
Geometry[angstrom]      10
C  0.0    -1.843324    0.133025
C  0.0    -0.613696   -0.391646
C  0.0     0.613696    0.391646
C  0.0     1.843324   -0.133025
H  0.0    -2.728775   -0.491109
H  0.0    -2.000484    1.20716
H  0.0    -0.495039   -1.473421
H  0.0     0.495039    1.473421
H  0.0     2.000484   -1.20716
H  0.0     2.728775    0.491109
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 24
174.2767          297.9228          518.5211

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538.7597          780.9904          899.0718
935.4151          936.3573        1000.6886
1003.8829         1057.4243         1226.5960
1314.7435         1319.7664         1415.4322
1473.2852         1652.9463         1705.8417
3121.7476         3130.9783         3134.5251
3135.1337         3218.8231         3219.2522
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
GroundEnergy[kcal/mol] 95.12
End
!-----h_c8h10_R1-1_p8-----
Bimolecular   R1-1_p8
Fragment      c8h10
RRHO
Geometry[angstrom]      18
C  1.6067261426   -0.1578630815   0.5373197472
C  2.6193617534   0.3584105162   -0.1619073791
C  -2.1172136187  -1.1273014368   0.1630287512
C  -2.6321754881  -0.0266516438   -0.3775683341
C  -0.365527089   1.0490868636   -0.3242181703
C  0.1753583058   -0.0590210976   0.1981796724
C  -0.661645434   -1.2836508077   0.5054183751
C  -1.8132661077   1.1917648926   -0.7004372892
H  1.8366334806   -0.7357347743   1.4324038017
H  3.6455561839   0.2525348373   0.1706915821
H  2.4561483663   0.8947297824   -1.0907046102
H  -2.7617823196  -1.9762170288   0.3744692832
H  -3.6940305649   0.018291519   -0.6029682868
H  0.266137365    1.9196388474   -0.4778835044
H  -0.2472829673  -2.1523637402   -0.0271468421
H  -0.5538440274  -1.5373881032   1.5710165398
H  -1.8964819753   1.4230928688   -1.7736702381
H  -2.2415250056   2.0724565865   -0.1987530982
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]      48
78.7737          122.1077          190.8701
249.2652         384.2806          399.1733
444.4725         547.1848          571.7707
654.7361         704.3440          745.4870
858.6712         893.1496          935.5575
938.9694         964.1448          977.1094
987.6937        1013.5777         1024.6341
1035.0387        1087.5724         1162.2175
1200.5327        1218.7528         1228.4262
1315.7947        1336.9569         1376.0196
1391.7622        1421.7770         1453.6309
1469.3905        1473.5203         1679.9115

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1702.6336          1745.8951          2969.2368
2973.8543          2977.8101          2982.9899
3107.2252          3133.7978          3134.0454
3147.3857          3157.1308          3216.7603
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
Fragment            H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]    1
0  2
End
GroundEnergy[kcal/mol]  72.42
End
!-----c2h3_c6h8_R1-1_p10-----
Bimolecular      R1-1_p10
Fragment          c6h8
RRHO
Geometry[angstrom]    14
C  1.4971925585    0.0    0.0
C  -1.4971925585    0.0    0.0
C  -0.6654493483    1.2544238413    0.0
C  0.6654493483    1.2544238413    0.0
C  -0.6654493483    -1.2544238413    0.0
C  0.6654493483    -1.2544238413    0.0
H  1.202512633    -2.1991276074    0.0
H  -1.202512633    -2.1991276074    0.0
H  1.202512633    2.1991276074    0.0
H  -1.202512633    2.1991276074    0.0
H  2.1716174134    0.0    0.8694182462
H  -2.1716174134    0.0    0.8694182462
H  2.1716174134    0.0    -0.8694182462
H  -2.1716174134    0.0    -0.8694182462
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm]  36
119.4133          384.8814          407.7280
543.0287          580.6654          634.3587
723.0839          856.4434          890.5913
945.5480          967.4960          974.3476
988.0221          1002.2933          1021.2120
1043.8541          1180.8878          1219.6759
1222.6682          1227.3136          1366.2973
1381.0629          1402.3369          1437.8849
1470.3201          1474.2206          1704.6666
1751.0625          2974.2343          2975.7460
2978.0315          2979.3178          3130.5125
3130.6030          3152.7541          3155.1253
ZeroEnergy[kcal/mol]      0.0

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ElectronicLevels[1/cm]      1
0  1
End
Fragment      c2h3
RRHO
Geometry[angstrom]    5
C  -2.6815309499   -1.8887734891   -1.1309235268
C  -1.725733176    -1.3518528792   -0.4241833636
H  -3.0692157655   -1.4200651964   -2.0332260024
H  -3.1437000229   -2.8401606701   -0.8523521394
H  -1.1628990858   -1.5707617651    0.4715150322
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]    9
712.2118             819.4319             921.7170
1046.2369            1391.3607            1651.0507
3037.2336            3133.0072            3234.0563
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]      1
0  2
End
GroundEnergy[kcal/mol]  76.96
End
!-----c2h2_c6h9_R1-1_p4-----
Bimolecular    R1-1_p4
Fragment      c6h9
RRHO
Geometry[angstrom]    15
C  0.8528082279    1.1813873314    0.0748703727
C  0.870278509     2.0488513014    1.0816092556
C  0.7946048026    -1.2932452945    0.0595108443
C  -0.0528382852   -0.0329827159    -0.0147368959
C  -0.9563737626    0.035969563     -1.2035717804
C  1.0290610812    -2.1478752658    -0.9316634305
H  1.5312308278    1.3099507378    -0.7660364668
H  1.5467068545    2.8961810883    1.0896732684
H  0.2071626874    1.9442944709    1.9354088568
H  1.2638388403    -1.458582191     1.0268200405
H  -0.6795686139   -0.0276042378    0.8964107005
H  -1.2516145443    0.9953693578    -1.6088532907
H  -1.4701776098    -0.8509213164    -1.5542077552
H  1.668204634     -3.0115777367    -0.7868144243
H  0.5990943509    -2.0162370927    -1.9186032952
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]    39
91.4488             102.0763             151.5444
282.2727            309.5824             324.5924
399.8698            501.8355             606.1827
661.4670            701.5559             858.6653

```

882.1087	947.0531	950.9948
1011.6122	1032.4954	1036.4145
1055.0042	1120.6049	1170.3619
1262.5524	1290.7926	1317.4967
1334.0982	1434.9875	1446.6355
1458.5733	1691.8655	1703.5403
2902.2510	3122.9814	3128.6933
3133.8452	3137.1656	3141.3907
3208.6191	3215.6094	3244.5377

ZeroEnergy[kcal/mol] 0.0
 ElectronicLevels[1/cm] 1
 0 2

End

Fragment c2h2

RRHO

Geometry[angstrom] 4

C 0.0 0.0 0.5990703976

C 0.0 0.0 -0.5990703976

H 0.0 0.0 1.6619081422

H 0.0 0.0 -1.6619081422

Core RigidRotor

SymmetryFactor 2

End

Frequencies[1/cm] 7

642.0679	642.0679	772.6955
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772.6955	2069.5209	3420.9272
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3523.7963

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

End

GroundEnergy[kcal/mol] 102.53

End

!-----c10h15_R1-2_ts5-----

Barrier R1-2_ts5 R1-2_rp1 R1-2_p2

RRHO

Geometry[angstrom] 19

C -2.7632571234	0.1571469344	0.0423940846
-----------------	--------------	--------------

C -2.1483007589	1.1503388853	0.6814434901
-----------------	--------------	--------------

C -0.6480447531	0.9762150499	0.6954109242
-----------------	--------------	--------------

C -0.4653244374	-0.4990416634	0.2584364729
-----------------	---------------	--------------

C -1.7863946645	-0.8655495355	-0.4877560837
-----------------	---------------	---------------

C 0.7772028323	-0.8233965887	-0.5301857715
----------------	---------------	---------------

C 2.6817585052	0.8300430443	-1.2064430982
----------------	--------------	---------------

C 1.8006383193	-0.0158873602	-0.7400650301
----------------	---------------	---------------

H -3.8316715077	0.0910210631	-0.1288955745
-----------------	--------------	---------------

H -2.6425859888	2.0144042211	1.1106620949
-----------------	--------------	--------------

H -0.195913904	1.1731581878	1.6717110131
----------------	--------------	--------------

H -0.1715405355	1.6668510173	-0.0118484945
-----------------	--------------	---------------

H -0.441637068	-1.1111006929	1.1697165116
----------------	---------------	--------------

H -1.6730701596	-0.7640629285	-1.575302053
-----------------	---------------	--------------

H -2.0927593344	-1.8991849716	-0.2982815523
-----------------	---------------	---------------

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H  0.8734238805   -1.8543916035   -0.8703169244
H  2.5131662422    1.3190462342   -2.1620148103
H  3.593179109     1.072755458    -0.6739522152
H  2.6721293469    -0.4125647511    1.0231900163
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  614.1488
WellDepth[kcal/mol]  58.08
WellDepth[kcal/mol]  4.3
End
Frequencies[1/cm]  50
49.0144          88.4920
121.7353         142.0216          309.2188
382.3188         397.4433          415.6475
463.7044         516.5044          621.3338
687.4386         716.0911          782.3093
821.3482         882.1313          891.4249
919.4426         945.2186          974.2290
976.0011         993.8873        1019.6210
1037.3035        1080.7254        1129.4359
1153.3684        1159.6756        1203.4786
1291.4682        1294.9107        1313.9378
1348.8363        1359.1796        1379.0064
1470.3008        1488.7840        1496.6983
1681.1756        1982.5204        2991.4467
3000.5172        3011.6512        3048.4480
3059.2323        3105.4959        3119.5302
3167.8644        3192.2819        3203.5366
ZeroEnergy[kcal/mol]  95.36
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-2_ts6-----
Barrier      R1-2_ts6  R1-2_rp1  R1-2_p3
RRHO
Geometry[angstrom]  19
C  -2.8206798667   -0.0512502028   0.2510098159
C  -2.2572114631   0.8310752908   1.0729844182
C  -0.7728756766   0.9750379791   0.8337754071
C  -0.490939857    -0.084507854   -0.2298427459
C  -1.8226880731   -0.6670265226   -0.6989408721
C   0.7018497355   -0.326102691   -0.8242442525
C   3.1261033487   0.0366233663   -1.0749941204
C   1.9568362923   0.301246434    -0.4734555615
H  -3.8741397509   -0.3038479745   0.2347338977
H  -2.7820836343   1.405004743    1.8273852776
H  -0.1848330505   0.8236779104    1.7448281622
H  -0.5237181694   1.9806583529    0.4670017607
H  -0.2044942984   -1.6141131614    1.1805348613

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H -2.0317073212 -0.377461781 -1.7382556739
H -1.8320658602 -1.7613533824 -0.6742118635
H 0.7390100415 -1.0678279382 -1.6199075598
H 3.197790347 -0.6883615799 -1.8797295331
H 4.0417043851 0.5355999851 -0.7818841753
H 1.9370948713 1.0335170261 0.3296327573
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 522.5111
WellDepth[kcal/mol] 41.11
WellDepth[kcal/mol] 3.58
End
Frequencies[1/cm] 50
73.8314 143.7359
147.8153 212.3315 353.0093
367.6424 372.7347 403.1387
446.7263 475.4737 667.4935
688.3536 698.3865 797.1621
817.6906 884.3156 925.2265
944.5404 951.7895 971.8163
979.3887 980.0836 992.2272
1029.7435 1112.1423 1131.8320
1166.2789 1185.2526 1219.4856
1291.9386 1293.9169 1323.4064
1343.1129 1379.4068 1454.7985
1467.0729 1473.6627 1631.7002
1663.2039 1687.4758 2991.0876
2992.4969 3038.9337 3042.6687
3124.2608 3132.9697 3145.2578
3176.9554 3200.7160 3221.6674
ZeroEnergy[kcal/mol] 78.39
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-2_ts7-----
Barrier R1-2_ts7 R1-2_rp1 R1-2_ip4
RRHO
Geometry[angstrom] 19
C -2.8686132319 0.1690048679 0.0134190628
C -2.2670318291 0.7717016397 1.0461250631
C -0.761649833 0.6860646847 1.1301948511
C -0.2696608878 -0.5624332091 0.4188871765
C -2.0515985205 -0.4494209827 -1.0275611944
C 0.9073579997 -0.6842058107 -0.2835421844
C 2.8704620349 0.203742182 -1.4754998811
C 1.7544638812 0.381690926 -0.7400199012
H -3.9548111384 0.1033216787 -0.038224642
H -2.8237736598 1.2875907273 1.82145407
H -0.4434430524 0.6537700681 2.1803865284

```

```

H -0.3011381527 1.5883433626 0.708488543
H -0.6978206963 -1.4820864797 0.807397074
H -1.5052710614 0.1854916764 -1.716032732
H -2.3374519595 -1.4166852308 -1.4321869481
H 1.2070574406 -1.6879480165 -0.5772264394
H 3.1987964553 -0.7866714736 -1.7745442766
H 3.4824921999 1.040017049 -1.7901990627
H 1.4791210113 1.3972613407 -0.4674231071
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 538.4421
WellDepth[kcal/mol] 31.31
WellDepth[kcal/mol] 31.78
End
Frequencies[1/cm] 50
72.1108 96.7353
158.3124 197.2498 292.9584
369.3742 380.6053 411.1913
523.7522 628.2245 638.2242
669.7502 727.9160 783.1424
831.6683 878.7220 895.7732
931.1228 945.9990 956.3098
974.8246 1009.8775 1020.9969
1027.3075 1076.5934 1160.4032
1184.0497 1222.5957 1255.6743
1310.7661 1325.6126 1379.0410
1390.2441 1462.2090 1469.9759
1480.4069 1535.0572 1613.7029
1652.4853 3000.2882 3020.8740
3104.4674 3113.4460 3122.9054
3132.3665 3142.3002 3148.7372
3168.8676 3195.5866 3222.2169
ZeroEnergy[kcal/mol] 68.59
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-2_ts8-----
Barrier R1-2_ts8 R1-2_ip4 R1-2_p5
RRHO
Geometry[angstrom] 19
C -2.8031060852 0.6755164398 0.296579458
C -1.7317494924 0.1978042028 1.165198294
C -0.4076214731 0.3358537937 0.9437831336
C 0.2653105825 -1.6503650303 -0.5804394464
C -2.6929696602 0.988651844 -1.0014976979
C 1.5100419347 -1.9428672321 -0.9081348677
C 3.9474026283 -1.5421351679 -0.8577289311
C 2.7040075277 -1.2074161717 -0.4995267783
H -3.7824679827 0.7565081136 0.7631543783

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```

H -2.0498794872 -0.3264350226 2.0630656401
H 0.3147576611 -0.0280737669 1.6627305023
H -0.0266170881 0.9439752686 0.1322975018
H -0.6933924691 -2.0955433215 -0.8022813233
H -1.7575665512 0.8852769715 -1.5408995496
H -3.5455271746 1.347494604 -1.5656103638
H 1.6884723421 -2.8162296042 -1.5475936975
H 4.1434213271 -2.4027256586 -1.4896863487
H 4.8058834005 -0.9677589825 -0.5314634441
H 2.5431280599 -0.3396262797 0.1337145402
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 169.2687
WellDepth[kcal/mol] 63.59
WellDepth[kcal/mol] 5.28
End
Frequencies[1/cm] 50
16.4898 52.3494
69.6074 79.1387 113.7529
185.6663 229.6526 295.3951
326.5765 514.1613 535.7931
568.7468 615.0591 754.0667
756.0255 814.1184 878.1835
889.2742 897.8028 933.5954
934.8901 955.0932 998.7197
1025.1237 1029.1801 1069.0662
1110.4877 1177.8554 1249.0613
1302.1431 1317.7108 1340.8795
1437.3293 1442.3862 1461.1912
1597.6178 1627.0070 1669.9319
1683.6665 3014.3554 3125.4347
3132.5126 3137.0811 3142.9952
3149.9484 3152.6843 3220.9658
3222.3088 3232.9712 3235.7269
ZeroEnergy[kcal/mol] 100.40
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-2_ts10-----
Barrier R1-2_ts10 R1-2_ip4 R1-1_ip7
RRHO
Geometry[angstrom] 19
C 0.798091623 1.6353265824 0.2981971272
C 1.2446503696 0.8583077924 -0.8417661418
C 1.3654556209 -0.4837317192 -0.883301736
C 0.9636532987 -1.4230975179 0.2359086216
C 0.1435462119 -0.7581111105 1.3124550929
C -0.7724541057 0.2631801215 1.0869508968
C -1.729909751 0.3950623775 -0.0220630307

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C   -2.0098234319   -0.5111089194   -0.9620100251
H   1.3424777922    1.5816622766    1.2320920309
H   0.3736933135    2.6166419744    0.0982128158
H   1.3975283059    1.4008219126   -1.7734391353
H   1.6935431116   -0.9522418887   -1.8063724152
H   1.8598393305   -1.8579428269    0.6969168364
H   0.4394023215   -2.2787796735   -0.2127425496
H   0.5267038147   -0.8431904061    2.3249752572
H   -1.0804708295    0.8089720435    1.9769074492
H   -2.2726650604    1.3376415264   -0.0392177893
H   -2.7486113258   -0.3061364875   -1.7282611824
H   -1.5346506097   -1.4832750576   -0.9934421223
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 568.1167
WellDepth[kcal/mol] 39.67
WellDepth[kcal/mol] 29.87
End
Frequencies[1/cm] 50
87.8374          127.1562
185.9232          228.3581          307.3296
376.4087          412.7326          444.5548
615.2171          642.0357          646.2157
688.1333          703.7718          803.4083
850.8333          862.1957          903.7339
921.6146          938.9042          951.2732
973.3601          1014.7951          1025.5731
1040.5468          1088.6769          1105.1786
1212.9356          1235.5430          1244.2227
1323.1840          1335.8706          1399.1337
1424.9020          1455.9284          1468.6438
1485.4645          1488.7325          1622.6415
1682.4448          2982.7307          3007.8378
3103.0546          3111.8164          3114.1651
3128.9673          3145.9934          3148.5913
3153.3052          3198.7866          3227.9167
ZeroEnergy[kcal/mol] 76.48
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-1_ts15-----
Barrier      R1-1_ts15  R1-1_ip7  R1-1_p8
RRHO
Geometry[angstrom] 19
C   1.7359126552   -0.350107185    0.3335031001
C   2.7703176972    0.1803210565   -0.3166759878
C   -2.0040483944   -1.2912993921   -0.0411801092
C   -2.5158448927   -0.1673584732   -0.5349546989
C   -0.2542608333    0.9125102478   -0.4254544486

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C 0.3116374392 -0.2718665645 -0.0725501925
C -0.5555835532 -1.4572964095 0.3232356966
C -1.7016671942 1.0735113395 -0.7751952253
H 1.9213581913 -0.906208877 1.2516932054
H 3.7788886422 0.103522251 0.0725324338
H 2.6444279124 0.6937747573 -1.2639437712
H -2.6479896855 -2.1515383545 0.118631571
H -3.5729264864 -0.1165475822 -0.7795423629
H 0.3841797351 1.7841835649 -0.5328119466
H 0.5030298687 -0.8689224529 -1.8701730809
H -0.1583157031 -2.3765125235 -0.1222877046
H -0.4627461983 -1.601795026 1.4110081578
H -1.7896612557 1.3798050204 -1.8300303072
H -2.1265259446 1.917166603 -0.2110133291
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 767.9592
WellDepth[kcal/mol] 31.54
WellDepth[kcal/mol] 5.73
End
Frequencies[1/cm] 50
82.5101 110.3248
186.1865 234.0494 389.5533
399.3637 419.1215 494.9329
516.8471 558.1350 571.7010
655.4471 695.6213 743.8725
828.9158 891.6837 932.5010
943.3335 963.5117 972.6847
978.0541 1010.0674 1016.2599
1036.9661 1084.4389 1153.0108
1201.7627 1213.7441 1232.0105
1313.6398 1336.0031 1373.9617
1388.7933 1421.0151 1449.9916
1461.0851 1472.5927 1618.1754
1691.2090 1734.4613 2961.0703
2970.1455 2980.0397 3025.9221
3113.5866 3136.1717 3137.4964
3155.2765 3160.3382 3219.1403
ZeroEnergy[kcal/mol] 78.15
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-1_ts16-----
Barrier R1-1_ts16 R1-1_ip7 R1-1_p10
RRHO
Geometry[angstrom] 19
C 1.1284653085 -0.1585296924 0.4712785821
C 2.3969827216 0.1048754558 0.2655707471
C -2.3412822812 -1.2964737168 -0.0997552259

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C -2.8324880721 -0.0595814976 -0.1366550207
C -0.8694632376 0.687974903 -1.5092818433
C -0.3011559822 -0.5334327878 -1.3539419968
C -1.072594449 -1.7087859795 -0.7958920026
C -2.1795441095 1.0709102447 -0.8854074764
H 0.5334829591 -0.1949145467 1.375940326
H 3.0876308268 0.3180305223 1.0850515983
H 2.8327082985 0.1220979436 -0.7319276187
H -2.8732926172 -2.0691171173 0.4487416409
H -3.7576995076 0.1678443968 0.3858224701
H -0.3233661855 1.466986227 -2.0325026833
H 0.6022508076 -0.7668724576 -1.9072366752
H -1.3148358764 -2.3979014928 -1.6196430134
H -0.4407617655 -2.2921458529 -0.1165633777
H -2.866533707 1.4480927557 -1.6588576838
H -2.0341771312 1.9296656926 -0.2114037466
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 348.0542
WellDepth[kcal/mol] 34.65
WellDepth[kcal/mol] 4.3
End
Frequencies[1/cm] 50
48.2957 67.0597
115.0305 161.4260 190.6370
299.1466 366.9863 400.4108
542.5236 581.0088 655.0895
733.0345 796.3707 845.9211
886.8430 889.4369 929.8113
934.2962 944.0295 967.1499
975.0777 988.4046 1010.7306
1049.1933 1085.6366 1175.5577
1209.8867 1215.6008 1219.1597
1363.3299 1372.2969 1397.1894
1398.3604 1434.5826 1464.6995
1477.0999 1589.3979 1642.1065
1729.1776 2965.2056 2968.3020
2971.1057 3025.8641 3048.0379
3127.2997 3132.6722 3146.0737
3155.7513 3165.4123 3193.2166
ZeroEnergy[kcal/mol] 81.26
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R1-1_ts14-----
Barrier R1-1_ts14 R1-1_ip7 R1-1_ip3
RRHO
Geometry[angstrom] 19
C 1.2432046422 1.260443384 0.4762940952

```

```

C  1.2435241151    2.0576106604    1.5405505956
C -1.3964026387    -1.0689120985    -1.2007818299
C -0.8785590181    -2.2718774385    -1.3313007511
C  1.2052320576    -1.2251269875     0.2099008322
C  0.3740392506     0.0341203095     0.3072556884
C -0.589552076     0.1859467435    -0.8995134301
C  1.3940566391    -1.9097876073    -0.9429055449
H  1.9162291225     1.4716681138    -0.3533350773
H  1.8962256575     2.9210456349     1.6051421671
H  0.5905463325     1.8736825196     2.3887263982
H -2.4753418465    -0.9298956235    -1.3193780316
H -1.3199262219    -3.2415619677    -1.5248384359
H  1.5213643866    -1.6672574454     1.1500149388
H -0.2433080413    -0.0607673009     1.2096561626
H -1.2620525375     1.0230155522    -0.6986787786
H -0.0135276996     0.4721799906    -1.788888463
H  1.9182787736    -2.8589685257    -0.9415969086
H  1.2617521023    -1.4533289136    -1.9153096272
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  403.998
WellDepth[kcal/mol]  40.39
WellDepth[kcal/mol]  9.08
End
Frequencies[1/cm]  50
87.6853          92.2972
206.6419         237.3333         290.6180
314.6950         377.8261         398.2692
518.6558         566.2361         647.4774
660.0299         706.7367         809.2677
841.5550         875.9210         918.4599
936.5920         944.7906         966.9331
983.4244         997.1662        1032.6818
1045.8443        1105.8699        1138.9604
1220.6946        1256.6230        1274.6144
1297.1603        1322.0219        1339.5116
1356.6425        1435.5659        1449.8152
1494.0876        1594.6700        1651.7138
1697.4143        3000.1190        3011.7947
3036.3583        3077.8409        3118.3372
3127.6827        3139.8559        3151.7646
3196.5956        3207.4482        3220.3289
ZeroEnergy[kcal/mol]  87.00
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-1_ts10-----
Barrier      R1-1_ts10  R1-1_ip3  R1-1_p4
RRHO

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Geometry[angstrom] 19
C -0.565922 1.360581 0.443915
C -0.280864 2.547394 -0.084988
C 2.481915 -0.082953 0.06533
C 3.358571 -0.886759 -0.212856
C -1.976079 -0.468319 -0.428531
C -0.541842 0.039627 -0.298674
C 0.399372 -0.943314 0.345842
C -2.482282 -1.569366 0.117828
H -0.860261 1.294316 1.490282
H -0.331415 3.457835 0.501884
H 0.008474 2.652244 -1.126545
H 2.110514 0.899223 0.267249
H 3.946079 -1.743933 -0.441327
H -2.620829 0.178629 -1.020794
H -0.191768 0.237705 -1.321842
H 0.432506 -0.990591 1.430008
H 0.554891 -1.888118 -0.161672
H -3.523169 -1.836846 -0.025541
H -1.882235 -2.241813 0.721107
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 470.4433
WellDepth[kcal/mol] 32.74
WellDepth[kcal/mol] 8.13
End
Frequencies[1/cm] 50
44.7270 72.5260
90.6545 105.6714 128.4700
226.1399 272.2776 311.6585
316.7503 407.3662 521.4969
533.9499 579.6176 648.0968
666.0414 696.0986 771.2382
777.7035 835.4070 872.9949
933.0545 949.6476 951.7183
999.8741 1018.0792 1034.7834
1038.9031 1138.4668 1183.2912
1280.6993 1307.5650 1319.5588
1338.4378 1438.5332 1450.1388
1460.3577 1689.3303 1701.2947
1892.8428 2985.3539 3117.1826
3120.1733 3120.7641 3128.5240
3137.1545 3208.0312 3214.6320
3215.6039 3347.1780 3459.5426
ZeroEnergy[kcal/mol] 110.66
ElectronicLevels[1/cm] 1
0 2
End

```

R1_secondary_c6h9

```
Well          rp2
Species
RRHO
Geometry[angstrom]  15
C   0.8437509359    0.9604783141    0.7729854028
C   1.5670660402    1.9073686626    1.3819587486
C   -0.20495359     0.0748761654   -1.3257446705
C   0.5269521747    0.9734296574   -0.6476094819
C   -0.8695548974   -1.1679090018   -0.7900192351
C   -0.3229094284   -2.4216099648   -1.395655044
H   0.4711275423    0.1303724266    1.3664916365
H   1.7848370785    1.8633602508    2.4422803345
H   1.9636943703    2.7569847806    0.8346501872
H   -0.3339448586    0.2312064941   -2.3939900439
H   0.936559286     1.813057982    -1.2055542041
H   -1.9473967655   -1.1097730338   -0.9901563709
H   -0.7801971782   -1.2064850793    0.3057852915
H   -0.9597388586   -3.2776234404   -1.5811260648
H   0.7424711487    -2.5278922135   -1.559294486
Core RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  39
47.3969           108.6574           130.4201
213.1922          258.7611           380.7756
436.9677          495.3619           607.4627
676.1322          793.6205           820.2181
908.8488          931.5385           987.4361
994.9143          1038.4625          1047.4122
1086.8052         1151.5663          1224.4669
1290.1770         1319.4203          1331.1399
1399.3067         1455.5816          1462.0681
1471.3704         1652.7846          1704.0838
2969.5175         3011.9325          3120.2458
3130.8462         3135.8492          3144.7430
3150.2230         3218.9507          3242.7186
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----c10h15_R1-1_ip5-----
Well          R1-1_ip5
Species
RRHO
Geometry[angstrom]  15
C   -1.4550003328    0.1112592369    0.0495192579
C   -0.7502779507   -1.1877746908    0.3203085353
```

```

C 0.6366670921 1.3516453577 0.0453294992
C -0.7432200032 1.2943194153 -0.0828373627
C 1.4392497138 0.1106868342 0.3161608008
C 0.7075665528 -1.1523516975 -0.1693377264
H -2.5373242218 0.1171994257 -0.0186086805
H -0.7704230365 -1.3994278334 1.4014279878
H -1.2870458719 -2.0184981538 -0.1507522604
H 1.1503980321 2.3040522307 -0.0261125827
H -1.2885959544 2.2133163827 -0.2790684761
H 1.637469119 0.0287331732 1.3969067363
H 2.4243824553 0.1823829029 -0.1576372423
H 0.7085620859 -1.1575183373 -1.2647899056
H 1.2407333203 -2.0503722465 0.1560984191
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 39
184.2874 253.4747 431.8898
501.6990 515.4015 603.1539
690.4036 728.0461 832.7735
860.8897 890.1284 954.6180
958.8088 1013.0606 1055.9898
1060.1141 1137.0428 1145.5058
1163.2554 1217.8483 1270.2328
1344.9107 1356.0003 1369.3209
1399.8939 1446.4173 1475.7361
1478.4553 1494.2907 1511.3871
2955.5757 2957.1887 3020.3246
3034.2036 3040.9961 3065.2716
3140.6539 3166.1320 3175.5553
ZeroEnergy[kcal/mol] -31.55
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----h_c8h10_R1-1_p9-----
Bimolecular R1-1_p9
Fragment c8h10
RRHO
Geometry[angstrom] 14
C -1.0170099592 -0.0351673813 -0.087810951
C -0.2979728105 -1.2959189738 0.33062008
C 1.0944174274 1.1777069224 0.0546716002
C -0.3491037355 1.1212371297 -0.195415517
C 1.82290763 0.0547820788 0.1120436325
C 1.1731071752 -1.2892811307 -0.1178371054
H -2.0913604147 -0.0718862047 -0.2373762248
H -0.348528886 -1.3753686889 1.4279570689
H -0.8057125515 -2.1816082912 -0.0613972185
H 1.5645243887 2.1487420442 0.1716108442
H -0.8694148627 2.0391229205 -0.4490823254

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```

H  2.8971197578    0.0967978428    0.2612097009
H  1.2319968278   -1.523047367    -1.192500812
H  1.7254340133   -2.0812499008    0.3956252273
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  36
195.0171          302.4735          480.3380
522.3152          572.5337          673.0370
761.3957          776.7351          852.7114
930.8907          962.5081          974.8938
989.2866         1010.4233         1041.7417
1068.9335         1173.2329         1190.5489
1201.7289         1268.4368         1356.2996
1358.9929         1401.0825         1437.4940
1470.6216         1481.4223         1638.2905
1703.0695         2959.5781         2972.3911
3058.6153         3059.1860         3146.4773
3153.1924         3168.2145         3177.6850
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0  1
End
Fragment          H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]    1
0  2
End
GroundEnergy[kcal/mol]  11.95
End
!-----c2h4_c4h5_R1-1_p12-----
Bimolecular    R1-1_p12
Fragment      c4h5
RRHO
Geometry[angstrom]    9
C  -1.4487222083    -0.4326185116    1.1031699213
C  -0.3744895678    -0.5882569411    0.3591530666
C  1.4230480216     0.2817445099   -1.0933344666
C  0.3337242867     0.4785109378   -0.345060996
H  -2.111970598     -1.0471459191    1.6924022963
H  0.0412467171     -1.5969553749    0.2444009964
H  1.8527839396     -0.7066696673   -1.2223110857
H  1.9181983615     1.1016381266   -1.5990951602
H  -0.0744509523     1.4789258396   -0.2334905721
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  21
178.7824          301.9654          513.7116
563.9794          727.3379          786.4375
862.8538          937.6451          948.6567

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1031.1551          1174.8299          1252.5578
1317.1948          1443.7437          1631.3541
1684.1465          3015.4742          3133.3427
3153.5072          3221.8621          3247.0440
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  2
End
Fragment      c2h4
RRHO
Geometry[angstrom]      6
C  0.0    0.6634900906    0.0
C  0.0   -0.6634900906    0.0
H  0.0    1.23462754   -0.9225248038
H  0.0    1.23462754    0.9225248038
H  0.0   -1.23462754    0.9225248038
H  0.0   -1.23462754   -0.9225248038
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm]  12
834.2929          972.9227          974.1218
1066.8559         1238.5875         1379.4650
1472.0483         1691.5384         3121.2072
3136.3255         3192.3844         3220.8390
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
GroundEnergy[kcal/mol]  32.74
End
!-----c10h15_R1-1_ts8-----
Barrier      R1-1_ts8  rp2  R1-1_ip5
RRHO
Geometry[angstrom]      15
C  0.9564650517    1.2192651834    0.7961486776
C  1.6231052733    0.0449863888    0.9649350219
C  -0.251563842    0.6421705145   -1.2807269867
C  0.2783316427    1.5531696977   -0.4410046402
C  -0.3289914815   -0.8575272882   -1.067742452
C  -0.228724126   -1.3437012489    0.3481224197
H  0.8107546137    1.8802522106    1.6473286674
H  2.0215468079   -0.4989140049    0.119211041
H  2.010540643   -0.2414437779    1.9364978049
H  -0.7252396439    1.0015108393   -2.190501058
H  0.1449848511    2.6065650985   -0.676715918
H  0.4312180992   -1.3531977816   -1.6874572782
H  -1.2907092671   -1.190028025   -1.4910174181
H  -0.9455512448   -0.9746731123    1.071893502
H  0.1751716229   -2.3316606941    0.5375516167
Core RigidRotor
SymmetryFactor 1.0

```

```

End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  407.2873
WellDepth[kcal/mol]  10.76
WellDepth[kcal/mol]  42.31
End
Frequencies[1/cm]  38
164.2156          246.7053
331.2428          402.6589          477.1506
510.6665          614.4281          707.2120
753.8300          772.0690          845.1303
860.4545          926.0601          950.1889
970.1882          981.0676          1046.8223
1085.8346         1088.9545          1224.3754
1246.1630         1282.8777          1338.8913
1411.0978         1447.2864          1462.5543
1468.8005         1572.2616          1649.9924
2953.4151         2995.5746          3120.8606
3129.0773         3132.1613          3143.5983
3149.7471         3224.6295          3226.1366
ZeroEnergy[kcal/mol]  10.76
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-1_ts17-----
Barrier      R1-1_ts17  R1-1_ip5  R1-1_p9
RRHO
Geometry[angstrom]  15
C  -1.3772893722   0.0026848577   -0.2345621884
C  -0.7703423295   -1.3032725394    0.2187092782
C   0.7024674088   1.1331222155    0.3290841129
C  -0.6720260841   1.1420637726   -0.1615197019
C   1.3978947704   -0.0203072176    0.4147387646
C   0.7530676251   -1.32899784    0.0100077048
H  -2.4130344567   0.0125907466   -0.5584337119
H  -1.00459253    -1.4397084603    1.2858844738
H  -1.2317568345   -2.1466863338   -0.3022024896
H   1.1665959573   2.0747438029    0.602245077
H  -1.1223335917   2.0904877182   -0.434960905
H   2.4002830632   -0.0323673892    0.8264996441
H   2.6855677826   0.3891311154   -1.3474215793
H   0.9747660508   -1.5149242637   -1.0495163462
H   1.1944145405   -2.1608571848    0.5653128669
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  325.0663
WellDepth[kcal/mol]  46.13
WellDepth[kcal/mol]  2.63
End

```

```

Frequencies[1/cm]  38
171.3594          210.5620
286.8025          330.5718          486.8824
519.2182          570.2333          685.7377
756.5188          797.6260          851.0279
927.3513          967.7889          974.3836
987.0038          1006.1312         1039.2123
1070.2553         1175.0550         1194.0210
1197.9162         1267.9509         1355.8380
1357.5960         1401.2997         1438.5325
1470.9293         1482.3717         1593.1993
1681.9024         2968.2016         2996.5947
3061.5067         3064.9041         3151.2883
3161.9853         3174.3007         3183.8979
ZeroEnergy[kcal/mol]  14.58
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R1-1_ts13-----
Barrier      R1-1_ts13  rp2  R1-1_p12
RRHO
Geometry[angstrom]  15
C  0.8893776731  0.2708780657  -0.2983028284
C  2.1257500648  0.7190885416  -0.5370190311
C  -0.9718679768  -0.0967703398   1.3106227477
C  0.2431277314  0.3273139277   1.0089036896
C  -2.5739216392  -1.1057167129  -0.1209944696
C  -2.1494174573  -1.2436250745  -1.3955377291
H  0.3056327896  -0.1660875303  -1.102037882
H  2.5707451354  0.6590993223  -1.5229597756
H  2.7316248812  1.1606191281   0.248399221
H  -1.5081735618  -0.0855181745   2.2511606255
H  0.8445952288  0.77133578   1.8116397717
H  -3.2076362299  -0.2751290751   0.1658539835
H  -2.5255237938  -1.9364467722   0.5728061365
H  -1.6099859461  -2.1260236423  -1.7211854773
H  -2.2943738995  -0.4587854438  -2.1294789822
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  290.3643
WellDepth[kcal/mol]  37.52
WellDepth[kcal/mol]  4.78
End
Frequencies[1/cm]  38
22.4493          100.8791
104.2407          193.8191          214.0644
339.0815          371.5594          550.3159
566.9095          756.2582          829.5816
857.5105          886.4214          888.8726

```

916.0792	934.6719	979.6572
1021.7964	1036.2563	1187.3551
1239.6177	1256.9863	1309.4324
1321.7978	1442.2904	1465.5455
1589.4489	1630.2784	1684.2669
3015.0306	3130.0679	3130.3957
3139.8076	3164.3945	3197.7692
3205.8736	3218.1789	3233.3603
ZeroEnergy[kcal/mol] 37.52		
ElectronicLevels[1/cm] 1		
0	2	
End		
!-----		
End		

R1_secondary_c5h7

```
!-----r1-3_rp6-----
Well          rp6
Species
RRHO
Geometry[angstrom]  12
C  0.7002153115    0.2843490193    0.9798752969
C  0.2502074535   -0.9301307528    0.2032432565
C  -0.9351407558   -0.7044779376   -0.70505908
C  1.8784644636    0.8457990836    0.906763262
C  -1.4609528823    0.4699770661   -1.0379588598
H  -0.0475821445    0.7093596836    1.6608150481
H  -0.0092026067   -1.7247780934    0.9164070483
H  1.0886908941   -1.3205698489   -0.3843587463
H  -1.3706461822   -1.6130009516   -1.1170634174
H  2.4035909977    1.6754620954    1.3560297507
H  -2.3121700592    0.5344571341   -1.706027953
H  -1.0568404897    1.4053205022   -0.6659956058
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  30
94.8582           149.5878           261.2712
397.3667           512.4018           573.0544
670.2951           779.9040           828.2481
907.5879           938.5203           953.1000
1031.0037          1045.8123          1109.2237
1207.1310          1275.5054          1326.0602
1348.6860          1444.8420          1467.7422
1678.3461          1706.4159          2996.6459
3011.7763          3040.5163          3122.1637
3137.3209          3216.2544          3239.3211
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----c2h2_c3h5_r1-2_p7-----
Bimolecular      r1-2_p7
Fragment          c3h5
RRHO
Geometry[angstrom]  8
C  0.0    0.0    0.4414918248
H  0.0    0.0    1.5297451707
C  0.0    1.2274571769   -0.1957824309
C  0.0   -1.2274571769   -0.1957824309
H  0.0    2.1546553362    0.3627527557
H  0.0   -2.1546553362    0.3627527557
H  0.0    1.2960812234   -1.2782433226
```

```

H 0.0 -1.2960812234 -1.2782433226
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 18
429.8649 531.6773 551.3484
785.3716 810.5065 936.5863
1012.9503 1037.0010 1207.5850
1270.2294 1423.3954 1511.2262
1517.2794 3126.8472 3133.4950
3139.8670 3231.6020 3234.4382
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment c2h2
RRHO
Geometry[angstrom] 4
C 0.0 0.0 0.5990703976
C 0.0 0.0 -0.5990703976
H 0.0 0.0 1.6619081422
H 0.0 0.0 -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 7
642.0679 642.0679 772.6955
772.6955 2069.5209 3420.9272
3523.7963
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 8.6
End
!-----c10h15_R1-3_ts3-----
Barrier R1-3_ts3 rp6 r1-2_p7
RRHO
Geometry[angstrom] 12
C 0.577296121 0.5438800792 0.9556025878
C 0.2956407737 -0.9415533636 -0.5512067222
C -1.1185374191 -1.0937480225 -0.6850729021
C 1.4236792044 0.3325074512 1.825693946
C -1.902004636 -0.3648909215 -1.5160506418
H -0.1623758731 1.2154313831 0.5665061267
H 0.8625579159 -1.7340474817 -0.0815758275
H 0.8292728917 -0.3832931669 -1.3138433484
H -1.5971599619 -1.8168184887 -0.0281667168
H 2.1811957626 -0.1369104866 2.4097246684
H -2.9758794949 -0.5017984267 -1.5489733592
H -1.4781072841 0.3706514447 -2.1928508109
Core RigidRotor

```

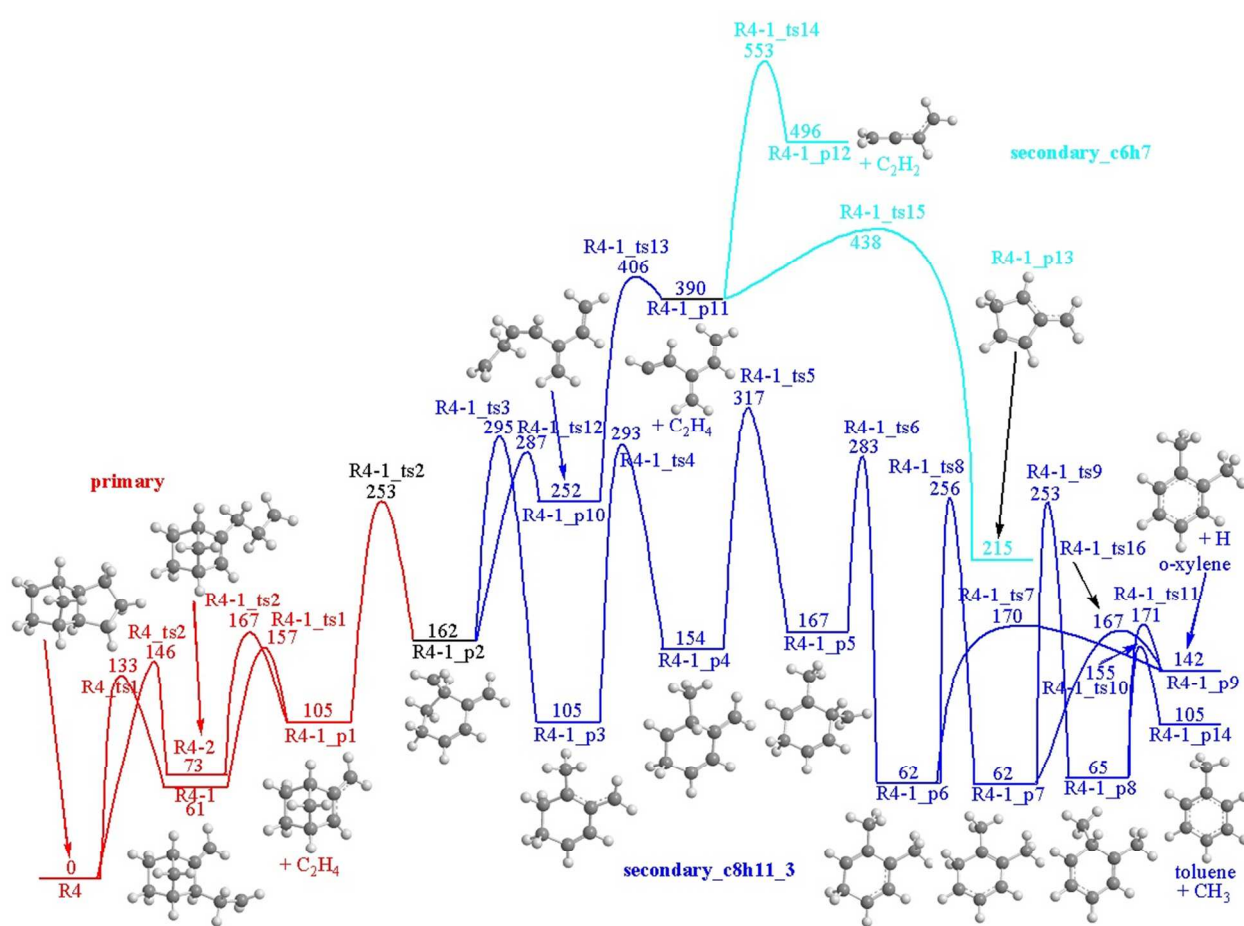
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SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 634.4105
WellDepth[kcal/mol] 25.1
WellDepth[kcal/mol] 16.5
End
Frequencies[1/cm] 29
59.7600          119.6770
237.6613          267.6017          424.8470
513.7371          626.6530          644.4337
729.8552          780.6337          834.1827
876.4923          949.3371          954.4618
1006.4305         1031.7590         1208.2999
1302.9527         1430.2699         1492.9646
1578.2726         1837.6106         3127.4201
3131.8441         3133.0533         3221.2411
3228.7582         3310.4708         3434.9461
ZeroEnergy[kcal/mol] 25.1
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```

Cartesian coordinates and vibrational frequencies of stationary points in R4 channel

Please refer to the following schemes for the notation of stationary points involved in R4 channel. Cartesian coordinates and vibrational frequencies of the stationary points are given below in the form of the corresponding fragments of the MESS input file.



Scheme S4. R4-1 and R4-2 channels.


```

C 0.0959221504 -0.1621929114 -2.5587657615
H -0.5423199971 0.8681923692 3.1274387805
H -1.8110116633 0.3504276946 2.0162254774
H -0.883988883 -1.8680612878 2.0527249265
H 0.3652012782 -1.3005909893 3.1571129249
H 1.6527629148 -1.8611491552 1.1019410608
H -0.6926674122 -1.7642553123 -0.2744447562
H 5.304632E-4 2.1307681867 1.0502433436
H 2.1304528331 0.6677214909 0.3714792147
H 1.9117702382 0.5891025513 2.1327172794
H 0.9310503113 -2.1354399539 -2.0101371938
H 1.9016997901 -0.753267174 -1.5020136767
H 0.487202575 1.8032778182 -1.6634555653
H -1.2149048046 1.5273875569 -1.9864635436
H -0.8083200456 -0.6623460113 -2.9213548571
H 0.6718887599 0.142845026 -3.4358715336
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
114.6505 154.9998 232.6991
279.3005 313.6119 382.4937
484.2982 536.3021 556.7802
617.9012 718.4824 736.2005
793.5710 822.2327 841.2685
872.5595 879.7906 887.4902
890.5442 903.0048 915.0810
955.4226 959.0434 988.0295
1013.0675 1037.1092 1042.3320
1058.0764 1089.7088 1121.8089
1131.4169 1149.4606 1162.8931
1189.5178 1205.5042 1221.5609
1230.0118 1246.5540 1251.0944
1281.7869 1302.3149 1307.7427
1311.2696 1322.8583 1335.2603
1338.1970 1349.1502 1362.9452
1472.4507 1489.2269 1490.8774
1499.8125 1505.8526 1521.2268
2955.9515 2978.4968 3012.7439
3021.5800 3032.7935 3034.4711
3034.7896 3045.7936 3070.0044
3070.9205 3079.9412 3080.2728
3084.7030 3090.6094 3093.8438
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R4-1-----
Well R4-1
Species

```

RRHO

Geometry[angstrom] 25

C	-0.8191005687	0.5646181397	2.4029099996
C	-0.3237612579	-0.9165600106	2.4738021647
C	0.5896172206	-1.0429582077	1.2308682635
C	-0.3090277913	-1.0454532364	-0.0379035305
C	-0.7901154565	0.4131227466	-0.0712431584
C	-0.1348787565	1.0992223529	1.1135593306
C	1.2244755602	0.3646495944	1.1744243801
C	0.4410838089	-1.4957603343	-1.3199263637
C	-1.6041319597	0.9786384129	-0.958004287
C	-0.4372962997	-1.7162608619	-2.5010800054
H	-0.4836765144	1.1365981611	3.2726535465
H	-1.9060214623	0.647900229	2.3503869847
H	-1.1464775197	-1.6356585314	2.4501907753
H	0.2426777216	-1.1002599645	3.3905911983
H	1.2822028807	-1.8855308829	1.27396949
H	-1.1559067459	-1.7272496098	0.1034516918
H	-0.1098889774	2.186988918	1.0398719854
H	1.8474662401	0.5339120366	0.2934798316
H	1.8044037461	0.6106338407	2.068515995
H	0.9574282186	-2.438418685	-1.0680911398
H	1.2270005641	-0.7757371746	-1.5648889138
H	-1.8615169202	2.031383279	-0.8936372482
H	-2.0349730444	0.416797299	-1.7793672729
H	-1.3229194375	-2.336315041	-2.4139991918
H	-0.177642249	-1.3432214697	-3.4831485259

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 69

61.3698	93.3404	116.1022
187.3247	214.7705	250.5572
333.1194	358.3647	410.5396
454.6874	503.3731	556.5340
647.7004	698.7300	726.6288
772.1507	780.2836	820.7871
856.9331	865.5305	888.8217
904.9544	915.9739	930.8309
945.8281	960.8722	992.4968
996.1276	1042.4533	1050.3298
1078.2958	1106.5371	1130.5109
1147.7230	1165.7471	1202.7202
1212.6661	1244.3548	1251.3051
1274.8689	1285.0412	1296.5135
1308.9080	1328.9861	1338.3453
1340.1213	1370.8843	1445.6627
1460.4734	1470.8789	1491.2959
1500.3732	1519.7628	1719.8132
2925.6887	3014.0632	3035.7727
3042.8840	3046.7762	3061.0200
3072.0505	3080.9767	3091.2448

```

3094.7157          3096.4438          3122.9050
3132.4627          3203.2695          3236.9339
ZeroEnergy[kcal/mol] 14.58
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R4-2-----
Well          R4-2
Species
RRHO
Geometry[angstrom] 25
C -1.122303766 0.5075856108 1.9896908264
C -0.7619074913 -0.9655129877 2.3589839223
C 0.6111130043 -1.1733505211 1.6332445656
C 0.3223972117 -1.1230711679 0.1398496563
C 0.0109163036 0.1414283438 -0.180728395
C 0.0964115635 0.9536320813 1.1115994848
C 1.2483306178 0.2208354905 1.8342174357
C -1.0405531785 0.3638351462 -3.9102160024
C -0.4663380689 0.7256960579 -1.4745189392
C -0.5685688512 -0.2622198824 -2.6442371164
H -1.1985173863 1.1334234521 2.88303205
H -2.0666920536 0.5906401898 1.4478855158
H -1.5114688259 -1.6833379743 2.0212533512
H -0.6485452801 -1.0874272768 3.4399364922
H 1.1778803798 -2.0360797708 1.9838461869
H 0.2692167539 -1.9939395514 -0.5016722845
H 0.1888776204 2.0336049566 0.9864649799
H 2.2069973036 0.3267690386 1.322616744
H 1.3555669891 0.5063486385 2.8857143801
H -0.8810015162 -0.123273817 -4.8643747283
H -1.6712702125 1.2454729423 -3.8933970646
H 0.1984909926 1.5528018324 -1.7589326647
H -1.4481662446 1.1939718511 -1.3124736932
H 0.4040028638 -0.7448939809 -2.8044442557
H -1.247135729 -1.0823887015 -2.3515524472
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
60.4580          80.3915          117.4823
135.4050          181.3369          251.8535
317.2717          358.7202          428.2362
475.0059          490.2335          542.6131
640.8414          730.0598          756.2304
785.8494          817.1249          825.8116
850.6975          862.4172          881.2355
897.5311          931.1416          950.5392
953.5909          970.8718          1001.7439
1039.4829          1053.0738          1078.8979

```

1090.5547	1126.0774	1140.0534
1149.3660	1176.1815	1189.9493
1207.2435	1237.9065	1252.6743
1283.2977	1292.0143	1303.6098
1306.1367	1312.8077	1328.2687
1346.9853	1402.7404	1463.5383
1468.7231	1478.5444	1490.5951
1493.1746	1514.4932	1676.3229
2926.0231	2984.5274	3001.7804
3018.0082	3033.4782	3036.8352
3049.0582	3076.8490	3086.4930
3092.8062	3096.7032	3098.7640
3131.7907	3192.5477	3232.5287

ZeroEnergy[kcal/mol] 17.45

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h15_R4-3-----

Well R4-3

Species

RRHO

Geometry[angstrom] 25

C	-1.8039583846	-0.9608974975	2.2874703624
C	-0.6968391031	-0.7075590322	1.3227433763
C	-1.0731708067	-0.9979403373	-0.1426003351
C	0.0944266312	-0.7927993161	-1.1490811259
C	-0.1259919984	0.6124493387	-1.6693352869
C	-1.3484866174	1.0605696587	-1.3938713885
C	-2.155960334	0.0062639134	-0.6615135766
C	1.587385208	-0.776389148	-0.7661209693
C	1.157325096	1.1819293212	-2.2201600506
C	2.2132066268	0.0823965659	-1.8940942531
H	-1.8318888383	-0.4644015081	3.2497626518
H	-2.5173848291	-1.7588448633	2.1128680993
H	0.1709422075	-1.3346181868	1.5910899207
H	-0.3453806066	0.3274712573	1.4195085719
H	-1.4474709988	-2.0255112004	-0.1918849762
H	-0.0274020754	-1.5069749541	-1.9787297401
H	-1.7421250782	2.0407638852	-1.6399129191
H	-2.7517352897	0.417523433	0.1603892466
H	-2.8648211542	-0.4906103557	-1.3379660842
H	2.0398945131	-1.7690552664	-0.6981243187
H	1.7315921789	-0.27894704	0.1976697574
H	1.4023430948	2.1297900982	-1.7305211375
H	1.1060914906	1.3872513224	-3.2937454327
H	2.3754756537	-0.5429497759	-2.7777254998
H	3.1835534139	0.4996216878	-1.6156098923

Core RigidRotor

SymmetryFactor 1.0

End

```

Frequencies[1/cm]  69
67.2252           102.4110           134.7638
151.2919           198.6726           235.2724
286.6789           339.7703           395.6668
449.9592           488.4834           561.6736
587.1808           672.3512           709.7774
770.1406           813.1719           818.8485
844.3807           853.6685           897.0012
905.8742           934.2658           964.5018
981.7003           995.3931          1015.2541
1029.4824          1077.4989          1086.0846
1106.9865          1153.2111          1172.6237
1176.6287          1189.8092          1223.4590
1235.6396          1256.5419          1263.9869
1293.7910          1308.5425          1318.5259
1320.8329          1335.9559          1351.8386
1362.9474          1390.2149          1460.2748
1468.7684          1478.9985          1493.6768
1494.0884          1508.9647          1725.1324
2927.8791          2955.1831          2990.6210
3014.7684          3028.2067          3033.3220
3034.8810          3037.4415          3041.4766
3056.6441          3076.0126          3087.6120
3129.0636          3172.3503          3229.7701
ZeroEnergy[kcal/mol] 17.67
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R4-3_i1-----
Well      R4-3_i1
Species
RRHO
Geometry[angstrom]  25
C  -2.1713123623   -0.9014626191    2.3614760614
C  -0.9243865334   -0.6871802336    1.4984481537
C  -1.1795242899   -0.8809728996    -0.0145218877
C   0.0902965862   -0.744646916     -0.9202117672
C  -0.1300804573    0.5326038803    -1.6910342891
C  -1.4231155797    0.9975396115    -1.4885607245
C  -2.1008820435    0.1798334531    -0.5953842063
C   1.5250045318   -0.5542923464    -0.3839789393
C   1.1640075334    1.1107191771    -2.1823156914
C   2.2324429515    0.1561849834    -1.5652261992
H  -1.9351896155   -0.7976677675     3.4240924083
H  -2.589001306    -1.9023017365     2.2111242289
H  -2.9540212859   -0.1753187009     2.1266243032
H  -0.1448205413   -1.3899439559     1.8140934522
H  -0.5281245092    0.3190494004     1.6713274997
H  -1.6163049691   -1.8806201006    -0.1357816671
H   0.1093452406   -1.596276433     -1.6186629271

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H  -1.8432598456    1.8910298891   -1.9374905821
H  -3.1314343576    0.3094602756   -0.2907485212
H   2.0213338596   -1.4871093258   -0.1036862502
H   1.5213384115    0.0981242031    0.4942877945
H   1.2950706165    2.1409786172   -1.828889292
H   1.2420673115    1.1494708689   -3.2755444812
H   2.5295132685   -0.5887910597   -2.3102066527
H   3.1393993851    0.6822017349   -1.2588478237
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  69
51.8016              103.4106              146.8224
184.9094              226.0990              232.4062
280.1055              332.3208              432.5272
494.5137              557.5690              578.1560
655.0691              676.9557              727.4318
752.2524              828.0916              841.7173
853.8809              888.0938              914.1301
919.5080              938.3492              957.6930
993.5355              1010.5962             1044.6854
1069.0929             1080.7279             1093.5073
1115.1233             1151.8703             1188.6515
1203.1888             1218.6706             1245.0048
1260.9766             1271.0769             1300.9599
1307.7943             1327.4194             1335.5802
1342.0829             1346.2808             1364.7936
1409.8804             1415.4635             1477.9552
1480.5460             1489.5954             1495.1154
1500.2191             1507.3436             1509.1524
2943.2769             2995.9529             3000.0656
3014.2382             3015.6608             3021.1985
3036.9890             3037.8399             3049.2308
3075.7498             3081.9590             3087.7680
3090.4154             3170.7600             3200.1230
ZeroEnergy[kcal/mol] -0.48
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----c10h15_R4-4-----
Well          R4-4
Species
RRHO
Geometry[angstrom]  25
C  -0.9605320899    0.3198048028    2.3430212082
C   4.208404E-4    -0.8756545115    2.2670330407
C  -0.3960224929   -1.8385886732    1.1314877857
C  -0.4786174183   -1.1121822046   -0.2367670177
C  -0.854060049    0.3518828198   -0.1430883008
C  -1.0685391483    1.001139152    0.9999799807

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C 0.4390741429 -3.0724520275 1.0965585619
C 0.7794378432 -1.029663473 -1.1315722594
C -0.684811764 0.9446901642 -1.5237866096
C 0.4132018964 0.0502213041 -2.1852512092
H -0.6044119324 1.0374445998 3.0895054282
H -1.9457439414 -0.0152784182 2.6971738349
H 0.007462125 -1.4205016242 3.2168308238
H 1.0196750911 -0.509780289 2.1004370162
H -1.4345822829 -2.1463925903 1.3606110926
H -1.253943686 -1.6192687657 -0.8317096432
H -1.2656551546 2.070578426 0.9842452673
H 0.4811133529 -3.6932456702 0.2093483381
H 0.8639409267 -3.4736878937 2.0098152236
H 1.0452946683 -1.9837622993 -1.5914933421
H 1.6351267198 -0.7059618356 -0.5307637188
H -0.4042833364 1.999319008 -1.4821873251
H -1.6188993441 0.8838593355 -2.093584201
H 0.0255185737 -0.4217041821 -3.0916497704
H 1.28685846 0.6339248459 -2.4821022045
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
63.2167 114.6773 124.2224
185.6202 225.2505 267.7106
304.7705 369.2158 428.7258
432.5300 493.4896 557.3221
604.1777 622.7574 694.3612
755.1747 777.0298 832.2525
851.7057 892.4494 903.2634
907.3687 922.6268 962.8603
1004.2860 1011.7592 1023.5392
1053.0330 1070.3312 1108.1380
1142.3223 1152.8390 1170.0632
1188.2217 1209.9150 1238.1033
1248.5114 1277.9152 1288.3152
1306.2567 1309.9472 1329.4789
1339.4829 1349.3464 1359.0671
1375.4007 1387.7722 1458.8585
1483.1193 1484.0230 1490.7456
1495.2876 1512.6933 1740.4355
2877.4991 2963.6091 2986.8886
3017.1764 3019.0608 3035.8566
3043.2220 3047.6291 3058.6930
3068.3969 3081.9429 3094.9645
3128.3094 3130.7927 3228.0736
ZeroEnergy[kcal/mol] 9.8
ElectronicLevels[1/cm] 1
0 2
End
End
!-----

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!-----c10h15_R4-4_i1-----
Well          R4-4_i1
Species
RRHO
Geometry[angstrom]  25
C  -1.0424114983    1.0385968774    2.217022901
C   0.0476301047   -0.0525105575    2.2791525943
C   0.0993690584   -0.8878396407    1.0372094576
C  -0.1566116673   -0.2389002366   -0.2884225317
C  -0.5689868912    1.2180567533   -0.2120224128
C  -0.9686204173    1.8010827376    0.9163684787
C   0.5916677801   -2.297339507    1.0853489864
C   1.0077536809   -0.1849170624   -1.3192805409
C  -0.3137213749    1.873809441   -1.5593455132
C   0.4943541102    0.8213256284   -2.36787204
H  -0.9258516915    1.7251397569    3.0616228607
H  -2.0305463658    0.5741122899    2.3360689762
H  -0.1061321289   -0.6924594084    3.1557222525
H   1.0174753144    0.4515880375    2.4434621796
H  -0.9716619947   -0.7939350885   -0.7926759396
H  -1.2244520527    2.8580512327    0.9252618237
H   0.1959487564   -2.8924019084    0.2545465817
H   1.6910307052   -2.3627582786    1.0178862976
H   1.2491214992   -1.1607677061   -1.7469548721
H   1.9078658233    0.1978368416   -0.8256721365
H   0.2518783911    2.8013403136   -1.4310340717
H  -1.244770097     2.141824466   -2.0686222161
H  -0.1631353527    0.3058505702   -3.0748031109
H   1.3014034739    1.2700158067   -2.9509253513
H   0.3091668345   -2.7920873585    2.0207453467
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
46.9317           101.5537           106.4253
163.3940          201.3514           252.0410
284.6918          346.2231           411.9529
435.7851          499.3096           553.6475
595.6790          650.5212           727.6749
798.7564          836.4754           853.2268
884.8486          895.2680           905.1692
917.8084          969.9444          1003.3720
1007.3509         1012.3444          1027.4206
1049.4360         1064.5105          1121.5909
1153.8693         1165.7004          1188.6300
1205.0279         1231.6191          1248.8374
1287.5845         1289.4498          1297.5340
1308.2955         1315.5717          1336.4573
1349.9324         1378.2942          1387.1732
1407.0886         1468.6488          1474.7645
1481.0458         1488.6731          1489.2799
1493.7484         1509.2125          1736.0871

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2883.0006          2904.9118          2934.2938
2993.0515          3018.9259          3023.9844
3026.6134          3026.9940          3035.6461
3045.1687          3055.9574          3063.6266
3078.9212          3087.8903          3130.0994
ZeroEnergy[kcal/mol] 3.11
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----c10h15_R4-4_i2-----
Well      R4-4_i2
Species
RRHO
Geometry[angstrom]  25
C  -1.010570118    1.0692385197    2.1888051632
C   0.0522957103   -0.0382068971    2.2832739741
C   0.1604256853   -0.8901936044    1.0000469202
C   0.2127275247    0.0083958777   -0.2059708581
C  -0.2612145556    1.3195386928   -0.1793513486
C  -0.8561944521    1.8836309328    0.9338008869
C   1.3473490201   -1.863649713    1.0853100118
C   0.7389040534   -0.3559037486   -1.5698330733
C  -0.0318696356    1.9788055559   -1.5290468624
C   0.2071046439    0.7808936089   -2.4780658696
H  -0.9533043767    1.7132330213    3.0733418752
H  -2.0151992761    0.6174743538    2.2189148139
H  -0.1542113438   -0.687573318    3.1402748109
H   1.0279897204    0.4286468869    2.4648974908
H  -0.7554055342   -1.5016970113    0.92317388
H  -1.2527534156    2.8931021049    0.9026028202
H   2.2934571562   -1.3191376126    1.1650605077
H   1.2553632244   -2.5064683215    1.9655740089
H   1.4048078705   -2.5104484516    0.2062527954
H   0.4090549936   -1.3458725095   -1.9066896011
H   1.8392231987   -0.3879220563   -1.5739863936
H   0.8518879568    2.6270249154   -1.4832691497
H  -0.870360299    2.6053359692   -1.8445870016
H  -0.7458612772    0.4719282329   -2.917559591
H   0.8845565255    1.0183525718   -3.3012812101
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
85.1282          132.6158          180.6504
208.1829          240.0247          249.8061
278.5031          401.2737          417.5571
434.0295          512.7467          556.7449
616.5616          632.0442          684.6082
725.2540          832.4919          848.4757
879.1350          895.8502          916.1893

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923.1899	954.5424	997.0014
1008.3517	1033.3847	1058.3167
1081.7231	1099.5200	1126.8203
1144.1604	1177.9749	1186.7643
1220.5620	1232.1433	1242.2789
1270.5461	1304.6159	1311.5932
1317.9892	1338.5972	1353.2021
1360.9176	1372.8418	1408.5317
1417.5967	1474.0477	1481.0933
1487.2209	1488.9595	1500.1002
1500.9630	1507.7117	1522.0876
2925.2933	2952.9475	2963.0148
3010.5118	3011.2952	3017.0065
3021.5805	3034.3522	3039.9806
3054.5728	3064.4561	3082.5189
3085.3291	3091.4503	3160.8029
ZeroEnergy[kcal/mol] -12.19		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----c10h15_R4-5-----		
Well R4-5		
Species		
RRHO		
Geometry[angstrom] 25		
C -1.7153463214	1.2327951502	1.626779673
C -2.5201541423	0.0043045355	2.1076067724
C -1.4745613587	-0.8934663548	2.6916710744
C -0.2750568009	-1.1321509352	-0.5466830856
C -0.2469373099	0.1371617521	-0.1283283406
C -0.3046289157	0.668547409	1.2819127932
C -0.0945249137	-0.4054120871	2.3800862837
C -0.2558815029	-1.2527254474	-2.0521042734
C -0.2059511218	1.0893093042	-1.3137023244
C 0.1441173252	0.1725118972	-2.5094175287
H -1.6199409047	1.9521089272	2.4463423592
H -2.1829950276	1.7520208381	0.7879267359
H -3.0350597533	-0.4784874931	1.2620288599
H -3.3073563024	0.2750959769	2.8220556335
H -1.6885795143	-1.776842906	3.2801879537
H -0.3462241949	-1.996993184	0.1026866033
H 0.4422914785	1.4657920405	1.3689206509
H 0.5952297199	-1.1974945636	2.0687875416
H 0.3703473211	0.0630598756	3.2639726873
H -1.2477362569	-1.5365992252	-2.4303601242
H 0.4397688827	-2.017988256	-2.4116425713
H 0.5214706305	1.8964755369	-1.1741943572
H -1.1818399697	1.5746959359	-1.449173112
H -0.3462086881	0.4756957318	-3.4369251236
H 1.2229046414	0.2048125414	-2.685556781

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Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
51.3994          93.9404          126.6874
149.7347        202.3956          249.2467
309.5042        342.3070          371.9001
502.7597        573.6516          645.0657
664.8660        758.9130          812.5439
822.8589        845.3930          862.2688
894.9359        904.4257          910.8323
915.2196        919.0263          940.4972
971.6995        995.1848          1035.1199
1040.4308       1053.7118          1063.0332
1115.3575       1138.4211          1150.6256
1175.4284       1194.8621          1226.7876
1233.3820       1254.7327          1275.7049
1288.1399       1306.5019          1316.3794
1326.5393       1339.2115          1344.6825
1362.5250       1394.6416          1470.8225
1475.7789       1485.4474          1491.1825
1500.2835       1510.1637          1698.8721
2930.7296       2951.3715          2989.7547
2995.2943       3009.3242          3018.2573
3029.9055       3031.5265          3037.7848
3040.7958       3050.8262          3086.7184
3088.2684       3180.2117          3190.5740
ZeroEnergy[kcal/mol] 8.13
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R4-5_i1-----
Well      R4-5_i1
Species
RRHO
Geometry[angstrom] 25
C -0.0848883066  1.960184432  1.0555011028
C -1.0964057059 -0.7072493234  3.5468078333
C -0.4520520717 -0.7374437318  2.3838104523
C 0.8599685832 -1.0821198997 -0.7400115111
C 0.9151208198  0.2177815899 -0.4342227168
C 0.9473993535  0.8805084096  0.9251801938
C 0.8925536928 -0.1108855581  2.1330099401
C 0.8592407513 -1.3320088857 -2.2301783697
C 0.9643620434  1.0634122441 -1.6975656706
C 1.2807298111  0.0400119427 -2.8130998982
H 0.051352352  2.7572871661  1.7770092561
H -1.058686144  1.8596858833  0.5923403859
H -0.6821862664 -0.2030075878  4.4152181878
H -2.0608318077 -1.1860265499  3.6755803434

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H -0.9132098905 -1.2492121093 1.5426902207
H 0.791022941 -1.8922140288 -0.0239666281
H 1.9330144751 1.3672806655 1.0000385664
H 1.6423963008 -0.8925884299 1.9560078329
H 1.2072146255 0.4273263735 3.0322180093
H -0.1419904967 -1.6286752981 -2.5716538718
H 1.5365647414 -2.1391144797 -2.527340923
H 1.7103871186 1.8627380975 -1.632538694
H -7.397457E-4 1.5595370388 -1.8605858938
H 0.7833488809 0.2722968108 -3.7570912671
H 2.357289945 0.0343922282 -3.0052748806
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
44.9845 70.5405 98.6688
127.1553 129.3810 174.1537
185.8554 243.8853 290.6406
352.8047 400.3044 483.7509
498.3084 565.7967 617.5192
643.2004 713.5297 815.3405
838.3023 852.3500 880.6666
902.9751 906.4638 916.9634
943.8537 963.2661 982.1641
996.8885 1035.3404 1039.2086
1061.3867 1091.4238 1130.8059
1140.6153 1169.1594 1222.2348
1230.2942 1243.0993 1260.4541
1292.1058 1316.7585 1325.4479
1328.1663 1346.4858 1351.5490
1369.4241 1451.6813 1458.7610
1484.4187 1484.7642 1489.9957
1509.4215 1698.9598 1705.1026
2953.3506 2991.8929 3006.2573
3007.0970 3031.6303 3040.8301
3052.0263 3057.6970 3087.5507
3121.8437 3133.0523 3141.8233
3186.0453 3205.9920 3237.4447
ZeroEnergy[kcal/mol] 27.25
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c2h4_c8h11_R4-1_p1-----
Bimolecular R4-1_p1
Fragment c8h11
RRHO
Geometry[angstrom] 19
C -0.7480168784 0.4461380072 1.5652472949
C -0.2963109615 -1.0466439883 1.6492103454
C 0.6468078167 -1.1927671543 0.4057072171

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C  -0.2219321609    -1.0590271797    -0.8201137362
C  -0.6383465515     0.2783330786    -0.9072004212
C  -0.0012667485     0.9713714605     0.2989403671
C  1.3325302795     0.1977758744     0.4085790584
C  -1.4774444143     0.8607988651    -1.8238023616
H  -0.4328906671     1.0042680385     2.450817577
H  -1.829606348     0.5561388334     1.4707765973
H  -1.1330267929    -1.746140816     1.6093251728
H  0.2595010194    -1.2452621363     2.5702359847
H  1.2943844668    -2.068879875     0.4387352466
H  -0.5604383355    -1.8746244119    -1.4469222903
H  0.0553953996     2.0576676896     0.2270901558
H  1.9889229298     0.3503671648    -0.4505007316
H  1.8808139087     0.4080342735     1.3319840198
H  -1.7333411179     1.9120804163    -1.7688290407
H  -1.901381844     0.2860978594    -2.6395404552
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  51
160.7614           249.4086           344.8050
388.0216           455.1904           541.0703
556.5269           623.9510           686.4251
725.1989           783.4013           798.5429
820.1372           836.7626           873.3434
881.6202           921.5896           938.1474
952.2232           963.6577           989.7240
1036.0866          1049.3634          1129.9936
1134.8773          1166.4914          1191.8440
1238.3811          1250.6178          1280.5289
1285.3558          1294.9792          1315.7410
1332.4062          1360.1192          1419.6271
1492.5268          1494.6820          1515.9188
1523.5593          3035.5863          3038.1308
3050.8281          3082.0073          3094.6958
3097.5385          3101.0784          3101.7777
3134.9457          3193.3579          3224.1973
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
Fragment          c2h4
RRHO
Geometry[angstrom]  6
C  0.0  0.6634900906  0.0
C  0.0 -0.6634900906  0.0
H  0.0  1.23462754 -0.9225248038
H  0.0  1.23462754  0.9225248038
H  0.0 -1.23462754  0.9225248038
H  0.0 -1.23462754 -0.9225248038
Core RigidRotor
SymmetryFactor 4

```

```

End
Frequencies[1/cm]  12
834.2929           972.9227           974.1218
1066.8559          1238.5875          1379.4650
1472.0483          1691.5384          3121.2072
3136.3255          3192.3844          3220.8390
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
GroundEnergy[kcal/mol]  25.09
End
!-----c2h4_c8h11_R4-3_p1-----
Bimolecular  R4-3_p1
Fragment      c8h11
RRHO
Geometry[angstrom]  19
C  -1.3041919299   -1.1811229235   1.0454971757
C  -0.0993392872   -0.9173711578   0.2017605849
C  -0.311163397    0.5137639149   -0.2492333448
C  -1.4772585662    1.0070032493    0.1652890297
C  -2.2688468496   -0.0281162048    0.9456488142
C  1.3390459637    -0.833249579     0.7764426893
C  0.9765806494     1.0873862254    -0.7773515486
C  2.0609743524     0.0933962149    -0.2381605862
H  -1.5517986602    -2.1369149183    1.4902938408
H  -0.062351725     -1.603955217     -0.6650007611
H  -1.8153797412     2.029703791     0.0409882724
H  -2.5795669404     0.3575518752     1.9293879556
H  -3.2095031922     -0.3132142022     0.4430335926
H  1.8292869915      -1.804329071     0.8794119593
H  1.3025735979      -0.3663831846     1.7655461492
H  1.1357591711      2.1078339685     -0.4196202577
H  0.995727081       1.1277263312     -1.8712707886
H  2.455452653       -0.5050566474     -1.0644918086
H  2.9101738289       0.6120785352     0.2116120319
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  51
94.5728           180.1562           233.7398
328.3175           363.0075           418.4472
558.1997           609.8309           661.1569
733.0000           788.3316           814.8693
832.8870           885.5632           897.3057
925.9003           935.1134           956.4175
982.7315           1003.1691          1041.1462
1061.2483           1127.2853          1130.1328
1156.5365           1181.0231          1226.9334
1258.9582           1270.5069          1285.7166
1293.9730           1310.6925          1334.1426
1335.3936           1360.5091          1463.8022

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1480.7496          1493.1603          1507.9252
1719.7058          2896.9889          2929.3938
2960.2053          3027.1120          3035.0643
3042.4400          3063.3227          3080.5449
3092.6024          3175.9033          3190.1978
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  2
End
Fragment      c2h4
RRHO
Geometry[angstrom]      6
C  0.0   0.6634900906   0.0
C  0.0  -0.6634900906   0.0
H  0.0   1.23462754  -0.9225248038
H  0.0   1.23462754   0.9225248038
H  0.0  -1.23462754   0.9225248038
H  0.0  -1.23462754  -0.9225248038
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm]  12
834.2929          972.9227          974.1218
1066.8559         1238.5875         1379.4650
1472.0483         1691.5384         3121.2072
3136.3255         3192.3844         3220.8390
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
GroundEnergy[kcal/mol]  34.42
End
!-----c2h5_c8h10_R4-3_p4-----
Bimolecular      R4-3_p4
Fragment      c8h10
RRHO
Geometry[angstrom]      18
C  -1.1908475658  -1.0247038028   1.2335618594
C   0.068957809  -0.8807650463   0.4270032769
C  -0.1433304425   0.4057146478  -0.3302867233
C  -1.3609462799   0.9007676327  -0.0389389848
C  -2.0234975117  -0.0143764811   0.9052258812
C   1.4717720971  -0.6396117137   1.0262391113
C   1.1597183697   0.9377710491  -0.8635739623
C   2.2223923867   0.0430979112  -0.1470635693
H  -1.4208400117  -1.8650917742   1.8747340872
H   0.1356175658  -1.7280798529  -0.2752543541
H  -1.773344949   1.8489200065  -0.3619071911
H  -3.0283228824   0.127598382   1.2854241286
H   1.9654651404  -1.5515521091   1.3700766545
H   1.3891192716   0.0416986344   1.8788393515
H   1.2852450034   1.994428705  -0.6099640055

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H  1.2439301196    0.8631914806   -1.9527853372
H  2.5866362635   -0.7232836597    -0.8382580441
H  3.0933116163    0.6113299905    0.1864618211
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  48
119.6533           215.6642           257.1968
386.6716           540.9349           565.4224
624.2645           669.8271           718.4686
766.6892           839.9621           842.7341
867.6236           896.8063           904.6781
950.6031           964.7501           985.6146
998.2568           1032.1818          1067.7182
1126.0814          1136.6386          1152.5975
1188.1450          1223.3941          1252.3273
1267.7190          1285.8703          1307.7835
1329.4884          1338.2318          1380.3626
1481.7482          1494.3745          1507.8410
1564.4256          1663.6238          2970.1151
3024.5550          3036.1934          3037.9222
3054.7178          3081.1203          3091.2800
3178.2106          3192.1525          3211.9854
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment          c2h5
RRHO
Geometry[angstrom]  7
C  -0.010005306   -0.6933107306    0.0
C  -0.0101278473    0.7943060179    0.0
H  1.0129896616   -1.1052065195    0.0
H  -0.505895822   -1.1011687976    0.8861725792
H  -0.505895822   -1.1011687976   -0.8861725792
H  0.0594570724    1.3509979137   -0.9263066322
H  0.0594570724    1.3509979137    0.9263066322
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  15
110.5914           477.0780           812.8964
980.4879           1062.3378          1191.6403
1400.9674           1464.8482          1482.5188
1482.9254           2942.1526          3034.0643
3077.4164           3137.9063          3237.5020
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol]  31.07
End

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!-----ch3_c9h12_R4-4_p1-----
Bimolecular    R4-4_p1
Fragment        c9h12
RRHO
Geometry[angstrom]  21
C  -0.9582382621    0.3502927489    2.2165318426
C   0.1057542412   -0.7510111558    2.3786704498
C   0.4697648518   -1.4037454718    1.0624943105
C   0.4007651553   -0.6928280864   -0.0680569725
C  -0.0935137187    0.6988059966   -0.0677634586
C  -0.7253973867    1.2106035078    0.9938721425
C   0.8083227282   -1.0627290634   -1.4815621613
C   0.1404258036    1.2891061465   -1.4408260337
C   0.1648212541    0.0412160301   -2.3547414393
H  -0.9924710468    0.9644332774    3.1212992953
H  -1.9546013163   -0.1111207173    2.1274354155
H  -0.2426371422   -1.49717914    3.0987210794
H   1.0189236829   -0.3140963028    2.8127836555
H   0.8564435219   -2.4189799696    1.0709668994
H  -1.1576063834    2.2069665903    0.9674472222
H   0.4971841561   -2.070102738   -1.7678948684
H   1.9008970991   -1.0246510325   -1.574737388
H   1.1160829965    1.791299327   -1.4733359642
H  -0.614055491    2.0239072347   -1.7301509569
H  -0.8617969644   -0.2426476416   -2.6067556021
H   0.7009742209    0.2090594598   -3.2912304676
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  57
125.8663          156.2024          257.2083
273.7134          313.7716          373.4803
502.9543          512.4421          597.5703
625.8573          686.4851          722.2231
813.5026          824.5342          855.8789
862.0783          878.2494          894.6054
913.5092          962.7481         1004.9051
1039.2010         1061.5701         1087.8079
1133.5168         1141.4226         1154.8957
1188.3964         1194.0281         1245.3853
1268.2932         1294.7178         1305.6318
1320.4942         1335.9163         1354.1894
1375.5358         1393.4264         1472.9560
1477.8737         1484.2088         1485.5429
1504.3134         1679.2163         1736.8797
2954.2819         2967.0324         3003.1905
3009.0949         3035.4553         3052.0921
3053.9314         3073.2449         3078.2776
3088.9618         3145.7341         3147.3711
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1

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```

End
Fragment          ch3
RRHO
Geometry[angstrom]  4
C  0.0   1.995E-7   0.0
H  0.0   1.0804553795   0.0
H  0.9357017515   -0.5402277895   0.0
H -0.9357017515   -0.5402277895   0.0
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  6
505.1501           1403.0831           1403.0885
3103.6402          3282.6573           3282.6683
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol] 22.47
End
!-----c3h5_c7h10_R4-5_p1-----
Bimolecular      R4-5_p1
Fragment          c7h10
RRHO
Geometry[angstrom]  17
C  -0.3787528254   1.7500391966   2.1244607993
C  0.2947988972   -1.3959279238   0.2621073983
C  0.0817570661   -0.0966084979   0.5286230583
C  -0.1135130451   0.4663046201   1.8555722695
C  0.4007339515   -1.6797118533   -1.2128398606
C  0.0140608895   0.7104741687   -0.7560314359
C  0.5564669245   -0.2658550735   -1.8292025666
H  -0.5171857568   2.0954034122   3.1420403715
H  -0.4686546847   2.4941961183   1.3408996778
H  0.3429866081   -2.1731523239   1.0176177049
H  -0.0378311389   -0.2379523911   2.6815886715
H  -0.5076652384   -2.1829615905   -1.5726174432
H  1.235981632    -2.3420294029   -1.4630054314
H  0.5973957512   1.6345065823   -0.7031756217
H  -1.0234536255   1.0059226645   -0.9583032826
H  0.0469430433   -0.1640631844   -2.7893949049
H  1.6168715512   -0.0624805214   -2.000877404
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  45
125.7464           138.3851           214.1687
255.5126           424.5906           473.4341
590.2620           645.5891           702.6531
820.3610           840.2892           878.7921
909.4662           915.2881           926.5998
959.4956           1024.0776          1026.6990

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1043.2056          1063.5893          1155.0422
1183.1114          1232.3629          1253.0723
1285.9671          1318.0419          1326.2700
1328.5397          1375.8261          1450.8716
1485.3599          1489.6195          1509.9747
1649.8478          1696.0898          2988.7571
3006.4366          3034.5863          3046.2867
3057.7809          3090.5166          3127.8436
3141.5245          3171.6667          3221.9748
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment      c3h5
RRHO
Geometry[angstrom]      8
C  0.0  0.0  0.4414918248
H  0.0  0.0  1.5297451707
C  0.0  1.2274571769  -0.1957824309
C  0.0  -1.2274571769  -0.1957824309
H  0.0  2.1546553362  0.3627527557
H  0.0  -2.1546553362  0.3627527557
H  0.0  1.2960812234  -1.2782433226
H  0.0  -1.2960812234  -1.2782433226
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  18
429.8649          531.6773          551.3484
785.3716          810.5065          936.5863
1012.9503         1037.0010         1207.5850
1270.2294         1423.3954         1511.2262
1517.2794         3126.8472         3133.4950
3139.8670         3231.6020         3234.4382
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol] 29.40
End
!-----c5h8_c5h7_R4-5_p2-----
Bimolecular      R4-5_p2
Fragment      c5h7
RRHO
Geometry[angstrom]      12
C  -0.2656633677  -0.9652976902  1.16731703
C  -0.2067301629  0.3321947403  1.391716896
C  -0.232916265  -1.2092153697  -0.3395776695
C  -0.1350663701  1.2296958135  0.1986997585
C  0.1573201039  0.1808974542  -0.9257934623
H  -0.3639857762  -1.7561730148  1.900151029
H  -1.2194429366  -1.5366685631  -0.6904753885

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H 0.4803249474 -1.9887235627 -0.6240163545
H 0.6441967477 1.9924882046 0.2698093377
H -1.0863476006 1.751679461 0.0436484055
H -0.3748362172 0.4110993295 -1.8507253425
H 1.2266548973 0.1923171972 -1.1479382395
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 30
138.1853 372.5103 615.9211
749.3413 761.8677 808.4759
875.3322 888.9709 925.7319
969.8009 1011.5459 1049.2739
1134.5420 1190.1466 1212.2706
1230.9245 1291.4628 1301.7688
1332.3079 1481.3588 1489.4274
1505.0024 1673.8528 3007.3214
3020.8374 3045.6554 3056.6088
3067.9027 3099.5445 3193.4524
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment c5h8
RRHO
Geometry[angstrom] 13
C -0.9590582092 -2.1713837036 -0.1801722802
C 0.9590582092 2.1713837036 -0.1801722802
C -0.0018870018 1.2527832294 -0.174266712
C 0.0018870018 -1.2527832294 -0.174266712
C 0.0 0.0 0.6668893539
H 0.9025969729 3.0499984902 -0.812951267
H -0.9025969729 -3.0499984902 -0.812951267
H -0.8823486242 -0.008511337 1.3179629254
H 0.8823486242 0.008511337 1.3179629254
H -0.8644546075 1.3771991382 -0.8263379051
H 0.8644546075 -1.3771991382 -0.8263379051
H 1.8375352291 2.079945644 0.4520385619
H -1.8375352291 -2.079945644 0.4520385619
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 33
88.4693 103.0923 301.3967
373.4141 453.4717 615.9070
680.2008 899.4987 913.3253
947.3083 948.6890 965.0603
1032.1956 1034.9737 1084.8443
1167.9590 1262.3906 1305.1039
1321.4261 1329.8601 1448.6147
1450.1292 1476.0799 1696.0347
1711.7911 3005.9649 3043.4491

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3120.8611          3120.9299          3129.1043
3129.7765          3207.4104          3207.4763
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0 1
End
GroundEnergy[kcal/mol] 63.81
End
!-----c10h15_R4_ts1-----
Barrier      R4_ts1  R4  R4-1
RRHO
Geometry[angstrom]    25
C  -0.7109721033    0.546374396    2.2885659168
C  -0.2610695035    -0.950277969    2.3646570347
C  0.6745232557    -1.1079047705    1.1398560296
C  -0.199431569    -1.0891033966    -0.1404807076
C  -0.6600950987    0.3596136209    -0.1694234825
C  -0.0052116836    1.0554241202    0.9982610779
C  1.3407295959    0.2869674487    1.0870292662
C  0.5697301348    -1.3531535409    -1.4986563405
C  -1.1077654553    0.890446963    -1.3454089905
C  0.5988989761    -0.1389633125    -2.39989122
H  -0.3609343078    1.1099571562    3.1583603122
H  -1.7948758304    0.6611915048    2.2325100619
H  -1.1056883673    -1.6427786964    2.3232339163
H  0.2793176587    -1.1521195345    3.2932256301
H  1.3479066827    -1.9645344011    1.2033683826
H  -1.0219639863    -1.8061093368    -0.05470894
H  0.0476198642    2.1417710915    0.9138447288
H  1.9825496166    0.4353717957    0.21600016
H  1.9104522422    0.5250948564    1.9900900657
H  0.0902008249    -2.1862688681    -2.0187437566
H  1.5892039651    -1.6846813744    -1.2668580062
H  -1.1796758968    1.9662641435    -1.4816509332
H  -1.7227199683    0.3014911883    -2.0169101977
H  0.2674244333    -0.2430198223    -3.4277151723
H  1.3902265203    0.5889497379    -2.2575858358
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 556.5698
WellDepth[kcal/mol] 31.79
WellDepth[kcal/mol] 17.21
End
Frequencies[1/cm] 68
70.1204          137.7848
229.1773          253.4771          338.7683
365.8122          452.7263          512.8584
525.8272          574.7823          665.6231
712.3699          743.4137          761.8569
785.9845          812.0392          821.8779

```

851.5674	868.8933	882.6350
898.8722	908.4191	922.4071
944.9100	957.4127	970.7596
985.2053	1029.7622	1046.3732
1050.6558	1084.5270	1126.8044
1135.5414	1162.3289	1205.9733
1219.5733	1241.4985	1247.7004
1265.8001	1280.3254	1282.8506
1294.8209	1312.0509	1322.9452
1340.0896	1347.2238	1428.5930
1468.5171	1489.9999	1490.9733
1502.3175	1520.4698	1573.7948
3009.7349	3027.4376	3034.0375
3041.3693	3045.8244	3065.6902
3072.0117	3082.3323	3090.1776
3093.5101	3095.8188	3113.9790
3119.5669	3187.6080	3206.8379

ZeroEnergy[kcal/mol] 31.79

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R4-1_ts1-----

Barrier R4-1_ts1 R4-1 R4-1_p1

RRHO

Geometry[angstrom] 25

C	-0.7407058193	0.6096332221	2.3186662914
C	-0.3419856752	-0.8965283801	2.4349784045
C	0.5441534162	-1.1245140757	1.1689892942
C	-0.3836123514	-1.0745865984	-0.0358846137
C	-0.8096527242	0.3199292577	-0.1317567832
C	-0.0656296714	1.0475086387	0.9843570121
C	1.2525263069	0.2456869002	1.0580767171
C	0.8071450946	-1.6247664419	-1.7544221474
C	-1.7104576665	0.8596043954	-0.9725651135
C	0.0280738708	-1.7484762273	-2.8774992224
H	-0.3380997318	1.1897597995	3.1537336402
H	-1.8208196665	0.7623224191	2.295908782
H	-1.2074455093	-1.5624958921	2.450849869
H	0.2362517021	-1.0886526874	3.3435366782
H	1.18193177	-2.0072839674	1.2315635377
H	-1.1005450799	-1.8722646963	-0.1931277109
H	0.0135318578	2.1270006808	0.8532630603
H	1.8751021532	0.3468548407	0.1679003521
H	1.8509888691	0.491379921	1.9396861183
H	1.1456159488	-2.5201617994	-1.2429585125
H	1.4611034075	-0.7663356934	-1.6623209749
H	-1.9556891821	1.9153434737	-0.9372693699
H	-2.2131304732	0.2594806787	-1.7226665196
H	-0.494073454	-2.6711574787	-3.105642579
H	-0.1729993924	-0.8997412894	-3.5204012101

Core RigidRotor

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SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 539.2102
WellDepth[kcal/mol] 22.94
WellDepth[kcal/mol] 12.43
End
Frequencies[1/cm] 68
45.1109          109.2640
120.4186          178.8545          245.6968
257.7135          345.1650          382.3159
416.7314          463.1344          551.0786
645.8009          671.4604          731.4239
774.1730          781.7853          812.3300
817.0529          827.5691          849.7081
867.0570          876.4014          885.6072
926.1926          943.3965          951.6327
964.3521          989.5620          994.1258
1012.7138         1043.0946         1053.4483
1129.8813         1138.8967         1170.4658
1198.4278         1239.2145         1241.9132
1247.5670         1264.2734         1275.9783
1280.3560         1296.2327         1318.7568
1332.2531         1338.3655         1439.3209
1462.9131         1489.8185         1500.0772
1519.9676         1549.5970         1630.0213
3033.1465         3045.4832         3050.8785
3076.3933         3087.1943         3096.4165
3098.5712         3104.9206         3120.6426
3131.5140         3133.9046         3166.1264
3201.1710         3214.7674         3228.2485
ZeroEnergy[kcal/mol] 37.52
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4_ts2-----
Barrier      R4_ts2  R4  R4-2
RRHO
Geometry[angstrom] 25
C -0.8205755922  0.5277642202  2.2483342919
C -0.4657434434 -0.9847861743  2.4119831341
C 0.6814780964 -1.1909607543  1.3674556384
C 0.0411648833 -1.0606815268 -0.0117027676
C -0.3058242391 0.2702902387 -0.1560850524
C 0.1410154193 0.9882133479 1.1018854187
C 1.4078035194 0.1691779138 1.4653147406
C 1.0624945864 -0.9372828257 -2.0309767342
C -0.6366180089 0.8391560842 -1.4994053881
C -0.1385065077 -0.1935716812 -2.5556612141
H -0.6126004952 1.0841869335 3.1669117409
H -1.8680266433 0.6917900231 1.9899591265

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H -1.3158346398 -1.6417018427 2.2164082596
H -0.1077099634 -1.2016010608 3.4223290108
H 1.2786656078 -2.0882756788 1.5294670623
H -0.4636170191 -1.9000299997 -0.4757690331
H 0.2553975802 2.0698754999 1.0170392165
H 2.2120565103 0.2759879942 0.7350727598
H 1.7908488221 0.3892679912 2.4667497878
H 1.2365255028 -1.9538761239 -2.3701365867
H 1.9649605681 -0.3647570208 -1.8366435818
H -0.1115604592 1.7958441685 -1.6214771522
H -1.7010888598 1.059566552 -1.6472519585
H -0.9401936322 -0.9080190091 -2.7709461823
H 0.0746424073 0.3194607309 -3.5025765367
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 490.1642
WellDepth[kcal/mol] 34.89
WellDepth[kcal/mol] 17.44
End
Frequencies[1/cm] 68
102.9205 155.9764
190.7239 262.0446 302.6421
397.3398 454.5099 504.9959
525.1677 564.7471 633.6727
715.7351 746.0007 785.2149
802.7794 819.5011 840.9117
855.3046 860.7701 869.8463
879.2462 922.3848 939.7134
947.7364 958.9786 977.6658
1032.5104 1034.7263 1050.8466
1070.4461 1118.0782 1136.8376
1147.4401 1173.7163 1190.6145
1205.5359 1216.7415 1238.4264
1248.5762 1279.4112 1294.5163
1303.9113 1318.5758 1326.7160
1342.4239 1363.2776 1459.7380
1471.4459 1489.9068 1492.9199
1494.1302 1503.5525 1520.9874
2992.4381 3002.2181 3013.9742
3034.6180 3036.8622 3043.7495
3047.4228 3077.1546 3088.0321
3094.3600 3097.8130 3100.3309
3105.9411 3161.4658 3194.8165
ZeroEnergy[kcal/mol] 34.89
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-2_ts1-----
Barrier R4-2_ts1 R4-2 R4-1_p1

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RRHO
Geometry[angstrom] 25
C -0.6636440935 0.8556436191 2.0070387362
C -0.6658808257 -0.5587236493 2.6669098629
C 0.2101773683 -1.4018814963 1.6768430495
C -0.5730842429 -1.5041436566 0.383433418
C -0.5931219632 -0.2694196421 -0.1976003719
C 0.2130437553 0.6436506236 0.728974137
C 1.2685215772 -0.347646373 1.2705700814
C -0.3563149615 0.4345039716 -4.1514473344
C -1.2424062222 0.1494881881 -1.3971084224
C 0.1947617223 0.0223562715 -2.9586411516
H -0.2034569622 1.5981935414 2.6644668256
H -1.6655049877 1.2092884099 1.7572132625
H -1.6689471723 -0.9747735159 2.7745850372
H -0.2065420398 -0.5361976353 3.659372238
H 0.5747523535 -2.3414783903 2.0921556336
H -1.1293497767 -2.3763008083 0.0605178013
H 0.5776034766 1.5670975601 0.2772754555
H 1.952232464 -0.7089444413 0.49967326
H 1.8414073152 0.0449439491 2.116733641
H -0.3530575573 1.4779568032 -4.4458907828
H -0.9108313194 -0.2495945645 -4.7838968964
H -1.4651240851 1.2037359992 -1.514195022
H -1.9817318077 -0.5148519054 -1.8307848281
H 0.9023717956 0.6722306267 -2.455066157
H 0.3504351892 -1.0360234852 -2.7827864731
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 614.0391
WellDepth[kcal/mol] 22.46
WellDepth[kcal/mol] 14.82
End
Frequencies[1/cm] 68
58.9580 76.0915
78.4867 193.8085 241.2729
252.4168 344.2332 413.7585
419.3200 471.7245 583.0322
613.0916 715.3014 742.0606
775.7909 787.0086 808.2376
815.6053 819.7345 842.8329
867.7563 877.5584 879.8171
926.9484 940.8796 953.4561
967.4436 1018.2862 1029.0868
1033.9768 1040.7404 1053.0816
1130.7689 1140.0199 1161.3450
1189.2377 1231.7198 1239.1200
1241.2077 1261.2441 1268.4487
1282.2418 1301.7022 1307.5222
1329.2591 1360.1970 1464.1323

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1480.1151          1490.7768          1493.9885
1512.0342          1525.4099          1558.6645
3034.7628          3036.8022          3049.7342
3080.8544          3089.8561          3093.5613
3098.7128          3099.7752          3119.5531
3125.0202          3131.6969          3184.6673
3194.2169          3209.5953          3224.3921
ZeroEnergy[kcal/mol] 39.91
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4_ts3-----
Barrier          R4_ts3  R4  R4-3
RRHO
Geometry[angstrom] 25
C -1.0911724146    0.1720528283    2.4919530978
C -0.3917287365    -1.1636506782    2.3594042687
C 0.7183722929     -1.0697965143    1.2647273657
C 0.0349227191     -0.8999288516    -0.115624351
C -0.2723751087     0.5747614651    -0.1523082553
C 0.2474626981     1.1963583648    0.9550716693
C 1.3532968887     0.3090519403    1.5190249749
C 0.7527544631     -1.0630945045    -1.4724775171
C -0.7213383606     0.9752996701    -1.5228758918
C -0.0961619726     -0.159470586    -2.4183616077
H -0.9128743973     0.7681003376    3.38102377
H -2.0777323071     0.2921173311    2.0606475373
H -1.0989802059     -1.9607705106    2.1037196123
H 0.0805462274     -1.4440090546    3.3066503474
H 1.4110991486     -1.9129000385    1.3204572888
H -0.8868244098     -1.503361783    -0.1529178826
H 0.2390115391     2.2706324705    1.1083772612
H 2.2756068801     0.4562514024    0.9434730948
H 1.5884521432     0.4792821951    2.5728025921
H 0.8027122818     -2.0969494622    -1.8252795542
H 1.7778375754     -0.6844890776    -1.4049504896
H -0.3678969578     1.9714271941    -1.8020547553
H -1.8135849301     0.9838139361    -1.6315104595
H -0.8932545276     -0.7517185012    -2.8759451353
H 0.5018924709     0.2519704266    -3.2340309808
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 507.8659
WellDepth[kcal/mol] 32.27
WellDepth[kcal/mol] 14.6
End
Frequencies[1/cm] 68
94.0989            153.3793
158.8169            225.4728            322.7879

```

363.1041	417.8247	517.1923
539.0582	578.2127	616.8900
685.6305	755.9068	764.5780
797.2327	817.2539	832.6671
860.7789	873.5890	887.5725
909.8347	929.8815	951.4978
971.3063	978.8884	993.8181
1027.7539	1037.7240	1061.8902
1092.5776	1131.4197	1143.3617
1158.8997	1186.7426	1219.9609
1220.7765	1250.0629	1254.9878
1270.5430	1280.6602	1297.9006
1311.1302	1321.6750	1329.5384
1352.9863	1367.7832	1465.0706
1481.2822	1491.0948	1494.7471
1503.2546	1511.1164	1527.2209
2941.3947	2992.8599	3011.5179
3012.7454	3028.0326	3043.8324
3049.7958	3055.7675	3066.2147
3069.3444	3070.9790	3091.1811
3122.5084	3164.4153	3212.3640

ZeroEnergy[kcal/mol] 32.27

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R4-3_ts1-----

Barrier R4-3_ts1 R4-3 R4-3_p1

RRHO

Geometry[angstrom] 25

C	-1.8720429178	-0.9642107721	2.2128742878
C	-0.80338971	-0.8144561333	1.3819007336
C	-1.403990991	-1.2087590543	-0.7620187667
C	-0.2206809441	-0.966651066	-1.675568665
C	-0.4324224016	0.4592835624	-2.1430833219
C	-1.6369365684	0.9200648131	-1.8100652886
C	-2.4417162991	-0.142699607	-1.0830472968
C	1.2669171332	-0.9531336019	-1.2533723922
C	0.8544378446	1.0354931904	-2.6777199104
C	1.9119333519	-0.0628973492	-2.3451645933
H	-2.5465332581	-0.142634455	2.4262491619
H	-2.1314316878	-1.9287282683	2.6353457896
H	-0.0578084246	-1.5980071971	1.313511133
H	-0.4732762147	0.1785656507	1.0974333096
H	-1.7379362159	-2.2241796693	-0.5773758417
H	-0.2968256868	-1.6559153656	-2.5385480279
H	-2.0130816871	1.9204652457	-1.9929409766
H	-2.9488066372	0.2417086613	-0.1896033531
H	-3.2435164377	-0.5501454143	-1.7218844271
H	1.7199526852	-1.9461869053	-1.2014404477
H	1.376733767	-0.4814857008	-0.2737735026
H	1.090108022	1.9833760698	-2.1846082477

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H  0.8136312056    1.2410143857   -3.7517724008
H  2.1058726817   -0.6665339135   -3.2373487434
H  2.8692333904    0.3577968939   -2.0299392121
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  430.5197
WellDepth[kcal/mol]  24.63
WellDepth[kcal/mol]  7.88
End
Frequencies[1/cm]  68
52.0479          87.6344
116.0963         152.4556         213.1508
235.8291         269.4696         353.1252
394.9180         406.8166         552.6547
592.1568         654.4490         707.4252
772.0259         808.5864         816.5959
827.1947         836.8181         848.5439
875.9638         900.2246         904.5155
936.0538         960.0681         977.2606
981.2431         1003.6308        1012.6743
1042.0471        1080.3174        1140.9243
1152.1655        1163.1904        1183.4315
1227.0061        1240.6058        1256.1810
1264.1251        1282.5054        1287.4442
1301.4783        1315.9127        1333.2384
1337.5002        1354.4631        1464.4125
1476.5578        1478.9996        1494.2386
1507.1819        1566.2373        1718.6324
2890.7517        2941.3135        3014.7796
3029.3085        3035.8252        3046.4072
3058.6071        3081.5179        3094.6628
3122.0678        3132.0804        3157.9758
3175.8200        3197.9873        3224.5576
ZeroEnergy[kcal/mol]  42.30
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R4-3_ts4-----
Barrier      R4-3_ts4  R4-3  R4-3_i1
RRHO
Geometry[angstrom]  25
C  -2.192308311   -0.4834493137   1.8928518819
C  -0.8803473341   -0.9512776922   1.2925919288
C  -1.1541620117   -1.2464240832   -0.2105960318
C  0.0057577997   -0.9127988437   -1.1832391964
C  -0.2969398083   0.5103915827   -1.6054059069
C  -1.5615420979   0.8625306654   -1.321115203
C  -2.2619336852   -0.2264400964   -0.6092588589
C  1.4955719377   -0.8452691144   -0.7986371273

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C	0.9504918597	1.1924883179	-2.1026184058
C	2.0686212339	0.1336022747	-1.8558866749
H	-2.1646334989	0.2873725478	2.6592409518
H	-2.944403548	-1.2493921202	2.0802523981
H	-0.4502369964	-1.8173225945	1.8077758912
H	-0.1516825163	-0.1401514577	1.3764397606
H	-1.4941952205	-2.2790873707	-0.3240927154
H	-0.0771752982	-1.5645869911	-2.0667229985
H	-2.0209572816	1.8175261938	-1.552475987
H	-2.6111237806	0.06061497	0.6316239565
H	-3.1951813325	-0.5993215212	-1.0373238227
H	1.9992272221	-1.8150081141	-0.8143550487
H	1.6200268101	-0.4237279407	0.2031320812
H	1.1388309042	2.1117419634	-1.5378144089
H	0.8911489449	1.4810347998	-3.1569399692
H	2.2666043234	-0.4115814957	-2.7841500904
H	3.0127836853	0.5852524341	-1.5433374043
Core RigidRotor			
SymmetryFactor 1.0			
End			
Tunneling Eckart			
ImaginaryFrequency[1/cm] 1798.6875			
WellDepth[kcal/mol] 16.75			
WellDepth[kcal/mol] 34.9			
End			
Frequencies[1/cm] 68			
97.1856	130.3825		
154.9668	223.7116	262.3055	
340.9560	414.8446	445.1645	
523.2858	584.8606	589.9127	
626.2414	689.0404	701.4563	
765.4433	822.2470	831.1649	
849.8465	874.4535	894.9863	
899.2070	908.7795	944.7023	
978.9057	989.8115	1002.6856	
1039.8463	1050.8427	1071.2148	
1084.3876	1106.1457	1157.7901	
1174.9420	1191.5520	1208.9516	
1223.1647	1252.0121	1256.0928	
1282.7038	1290.5184	1304.8715	
1312.3565	1335.4310	1343.4376	
1361.2657	1366.9282	1400.1980	
1458.0453	1476.4310	1489.8273	
1494.7076	1507.3808	1610.3584	
1655.2496	2959.4051	3021.8211	
3023.4561	3031.9888	3038.8752	
3047.2420	3051.1154	3066.1068	
3072.7910	3077.9460	3083.0774	
3089.3716	3166.6730	3170.6747	
ZeroEnergy[kcal/mol] 34.42			
ElectronicLevels[1/cm] 1			
0 2			

```

End
!-----
!-----c10h15_R4-3_ts5-----
Barrier      R4-3_ts5  R4-3_i1  R4-3_p4
RRHO
Geometry[angstrom]  25
C  -2.1330961861  -0.9083783185  2.1615425111
C  -0.8321094579  -0.695255324  1.4591664668
C  -1.3351675423  -1.1867936592  -0.8827460718
C  -0.0566102659  -0.9738966691  -1.6667540287
C  -0.2661089467  0.3661100585  -2.3223778465
C  -1.5305772576  0.7898518971  -2.0898507216
C  -2.2148456119  -0.2019455412  -1.2767699718
C  1.3778905598  -0.8519613721  -1.1172221854
C  1.0420023723  0.9592001016  -2.7696059526
C  2.0935889657  -0.0663062273  -2.2451040224
H  -2.0567077259  -0.697705487  3.2396942955
H  -2.4823220167  -1.942078681  2.069968368
H  -2.91464067  -0.2516649487  1.7676392702
H  -0.0465503039  -1.4325137156  1.5888891798
H  -0.4944418861  0.3225064537  1.3000058136
H  -1.6321698558  -2.150148293  -0.4915969395
H  -0.0494358456  -1.7502302568  -2.4521763134
H  -1.9667182957  1.7307386895  -2.4037215425
H  -3.2608378917  -0.1498840804  -1.0004025512
H  1.851981937  -1.8138419242  -0.9076657112
H  1.3761433202  -0.2695210769  -0.1929027197
H  1.1954487866  1.9470564399  -2.3218121282
H  1.1115628851  1.0946284415  -3.8541308791
H  2.3664464817  -0.7562220712  -3.0501571705
H  3.0154424516  0.4113795644  -1.9063381489
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  341.9787
WellDepth[kcal/mol]  37.29
WellDepth[kcal/mol]  5.74
End
Frequencies[1/cm]  68
46.0288          79.2707
99.1490          147.8792          163.4001
179.6231         227.3338          264.9487
403.5326         466.9297          517.7696
557.3115         606.9672          664.0740
701.8180         740.5067          776.7559
826.3996         837.7580          845.4442
871.8799         885.3835          901.4513
907.1184         962.6929          986.2397
1005.9559        1007.6898         1030.2475
1062.2605        1076.0769         1102.6728
1141.9026        1156.1498         1187.4529

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1212.6178          1223.9448          1250.5063
1266.1408          1293.0681          1311.0233
1330.1574          1336.3165          1379.0253
1400.9213          1439.9841          1469.2289
1480.2999          1484.1639          1488.5768
1494.8362          1507.9691          1621.1664
2947.5271          2961.8463          3019.1691
3029.8986          3033.4445          3045.5203
3049.3758          3074.7357          3081.4021
3096.0379          3118.4437          3178.7073
3191.1342          3207.4374          3212.9127
ZeroEnergy[kcal/mol] 36.81
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4_ts4-----
Barrier      R4_ts4  R4  R4-4
RRHO
Geometry[angstrom] 25
C -0.8462262202    0.3447284654    2.3455215564
C -0.2328485905   -1.0861723439    2.3400971204
C  0.7758804313   -1.1142403609    1.1756017978
C -0.0425248229   -0.9991729361    -0.1410753507
C -0.5218606012    0.4451383359    -0.1441173658
C -0.4337770527    1.0813726864    1.0779958052
C  1.5829936949    0.1541824735    1.3205696426
C  0.7142067176   -1.1232125212    -1.4840275827
C -0.3803225715    1.0537028832    -1.5186227167
C -0.0233509401   -0.1484900124    -2.4229679434
H -0.5125070732    0.9086724499    3.2200955933
H -1.9393704713    0.2994592659    2.4045366596
H -0.9978823768   -1.8566128012    2.2101401094
H  0.2696065791   -1.2887164384    3.2901935479
H  1.3812247362   -2.0292854537    1.1938814155
H -0.8609221292   -1.7312087886    -0.1235239776
H -0.4522451915    2.1687982399    1.1188700194
H  2.1963917197    0.4972398328    0.4937274367
H  1.9707617577    0.4061849063    2.304168171
H  0.7334645777   -2.1482504633    -1.8625419935
H  1.7540239045   -0.8021495216    -1.3609454336
H  0.4273072158    1.8002497398    -1.5272710245
H -1.2848915347    1.5736792787    -1.8507745969
H -0.9414506587   -0.617417539    -2.7925517843
H  0.5698819002    0.1354846226    -3.2952911055
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 555.7794
WellDepth[kcal/mol] 25.81
WellDepth[kcal/mol] 16.01

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End
Frequencies[1/cm]   68
116.8999           154.8399
230.4699           277.8242           327.2661
367.2273           444.2923           527.7102
535.0347           577.5858           599.6575
671.2402           737.2828           777.0109
785.7997           815.7843           853.1469
868.3091           886.1174           893.1819
907.6061           916.8487           946.6559
968.1105           1002.5396          1020.6428
1035.3041          1056.2816          1076.9243
1091.9525          1121.3534          1155.7212
1171.6587          1187.7378          1218.5117
1236.2438          1247.2110          1268.3972
1274.3628          1305.4252          1310.5528
1320.1034          1335.6310          1342.5521
1353.6453          1356.7008          1465.0430
1477.8285          1487.2083          1494.9172
1506.6468          1509.3260          1517.4304
2976.6726          2988.9060          3007.8397
3020.2527          3024.6246          3031.4214
3039.5815          3041.0891          3055.5319
3074.9456          3078.3213          3083.9717
3107.4262          3127.3892          3195.3793
ZeroEnergy[kcal/mol] 25.81
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-4_ts1-----
Barrier          R4-4_ts1  R4-4  R4-4_i1
RRHO
Geometry[angstrom]  25
C  -0.8519636455   1.0812377159   2.281522986
C   0.1786695056  -0.0619485244   2.2503371168
C  -0.0080517794  -0.9501349914   1.0500289148
C  -0.2241707595  -0.2935598223  -0.2910679004
C  -0.6434780425   1.1596994028  -0.1990341007
C  -0.9158279982   1.7830648786   0.9460056421
C   0.485236596   -2.3613717669   1.0977032281
C   0.9833927714  -0.1918309943  -1.2632114022
C  -0.486099477    1.7785404067  -1.573612896
C   0.504046308    0.8303844815  -2.3196055995
H  -0.5853168238   1.7998350284   3.063513667
H  -1.8365908113   0.6808661363   2.5580803752
H   0.1179265227  -0.6552299613   3.1690544433
H   1.1914654818   0.374338734    2.2339838749
H  -0.7586798747  -1.9764730899   1.2732482659
H  -1.0116850402  -0.8397717964  -0.8381743058
H  -1.1495428385   2.8451989652   0.9395943314
H   0.6275968569  -2.9095749131   0.1764779122

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H 0.9345969013 -2.7355188758 2.0078146043
H 1.2644115415 -1.1520030373 -1.7016028255
H 1.8518447819 0.1922985741 -0.7180978661
H -0.1105363286 2.8023197228 -1.5051249565
H -1.4452723746 1.8281946369 -2.1003451001
H -0.0119391049 0.3098238784 -3.1312642904
H 1.3351936315 1.3755752114 -2.7714551189
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1907.3232
WellDepth[kcal/mol] 35.13
WellDepth[kcal/mol] 41.82
End
Frequencies[1/cm] 68
53.7801 121.3652
167.3562 209.9501 256.6279
292.6205 369.2560 384.9605
425.5142 445.6616 537.4251
559.2359 611.2286 675.7369
688.7320 741.8072 783.1013
835.7403 849.8745 894.3565
900.2095 905.2227 917.5980
972.5492 1008.9817 1010.5431
1028.9486 1049.8299 1067.0186
1134.0199 1154.0446 1177.6232
1192.2181 1212.3686 1233.1450
1245.9207 1262.0710 1286.2436
1294.8788 1306.8094 1320.5450
1331.5740 1334.3201 1357.1247
1380.9306 1394.0986 1420.8922
1477.1736 1481.2970 1487.2745
1492.9742 1510.3387 1738.9198
2180.6891 2927.3389 2937.9937
2995.5085 3021.4889 3032.2792
3038.4243 3042.8248 3043.6826
3063.6325 3080.7604 3092.0503
3130.2843 3139.8659 3254.7574
ZeroEnergy[kcal/mol] 44.93
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-4_ts2-----
Barrier R4-4_ts2 R4-4_i1 R4-4_i2
RRHO
Geometry[angstrom] 25
C -1.0373044887 1.0918361403 2.1915109801
C 0.0063409397 -0.0403742828 2.3267629578
C 0.2146478036 -0.8316424483 1.062407309
C 0.0947295011 -0.0525351519 -0.2021621456

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C	-0.3250033754	1.3384442277	-0.166718389
C	-0.8439384765	1.9115224252	0.9410194722
C	0.9874024475	-2.1154185305	1.1075534002
C	0.7513632211	-0.3507622963	-1.5367849514
C	-0.0689913094	1.95444535	-1.5301285601
C	0.1553958724	0.7377235273	-2.4569091667
H	-0.993476931	1.7289784984	3.0811655042
H	-2.0429831985	0.6435989135	2.1960850867
H	-0.2681403418	-0.7054302092	3.1530195788
H	0.9719868074	0.4160085915	2.6045113805
H	-0.8364352245	-0.8303866852	0.165168655
H	-1.1721413245	2.9459006801	0.9362707379
H	2.059200847	-1.9303178227	1.2862177177
H	0.6369915352	-2.7650538889	1.9157131577
H	0.9138236101	-2.6756475396	0.1721582726
H	0.5684130012	-1.3610707924	-1.9114676472
H	1.8422220197	-0.2343202435	-1.4549222654
H	0.8366674699	2.5732023574	-1.4944990466
H	-0.8832640927	2.6004776951	-1.8693115803
H	-0.8060487153	0.3918216704	-2.8489152714
H	0.7976024023	0.9659508144	-3.3104431867
Core RigidRotor			
SymmetryFactor 1.0			
End			
Tunneling Eckart			
ImaginaryFrequency[1/cm] 1861.9631			
WellDepth[kcal/mol] 31.55			
WellDepth[kcal/mol] 46.85			
End			
Frequencies[1/cm] 68			
104.4900	153.6490		
156.7933	184.4874	239.6269	
253.3874	296.6027	359.5043	
408.0831	439.9713	515.6994	
554.7191	597.3982	631.5165	
705.7653	754.9162	833.2864	
859.6017	880.1948	893.0120	
915.1060	916.4981	980.5082	
1002.6907	1022.2119	1045.0144	
1054.1739	1059.1224	1120.4322	
1141.0063	1165.8103	1179.4601	
1198.4680	1227.9537	1229.8025	
1244.8419	1271.6303	1302.3720	
1312.3790	1326.3836	1337.0550	
1348.5290	1377.9373	1410.7077	
1426.9277	1476.2574	1480.2660	
1483.6147	1485.6044	1489.6644	
1498.1203	1506.7477	1626.1806	
2097.9659	2930.7712	2945.7024	
2963.2746	2972.4620	3004.6797	
3031.8464	3033.7943	3038.6528	
3040.6693	3058.5170	3062.3869	

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3085.5488          3088.7988          3156.1467
ZeroEnergy[kcal/mol] 34.66
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-4_ts3-----
Barrier          R4-4_ts3  R4-4_i2  R4-4_p1
RRHO
Geometry[angstrom] 25
C -0.3693230279 1.0190884426 2.2417683077
C -0.7620105182 -0.4502661653 2.0024535118
C -0.1445990922 -1.0313339211 0.7462011065
C 0.0510274652 -0.2097957282 -0.3178665587
C -0.1379383975 1.2352214906 -0.2114938455
C -0.3691434671 1.8342892409 0.968632005
C 2.16986146 -1.5613512163 1.5492785294
C 0.4302622783 -0.5543729994 -1.738544211
C 0.0121132635 1.8503372533 -1.5902645361
C -0.1188222271 0.6436046305 -2.5490805661
H 0.6355800255 1.0637149642 2.688112946
H -1.0424226979 1.4616024174 2.982640491
H -1.8557631792 -0.5164202061 1.892775988
H -0.507640529 -1.0505914209 2.8793630397
H -0.1873308768 -2.1060598872 0.6089105826
H -0.4866849573 2.9118497517 1.0396004471
H 2.5208467686 -0.5662614332 1.7860287286
H 1.8835961983 -2.207767432 2.3690448501
H 2.5477551648 -2.0259693991 0.64829242
H 0.03519714 -1.5175910919 -2.0708869306
H 1.5240532914 -0.6036397639 -1.8354972973
H 1.0073702226 2.3019753061 -1.6875392327
H -0.7183177858 2.6377623194 -1.7904907448
H -1.1751628459 0.4712886722 -2.7777851549
H 0.4041833236 0.7934941755 -3.4960488759
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 319.8646
WellDepth[kcal/mol] 39.68
WellDepth[kcal/mol] 5.02
End
Frequencies[1/cm] 68
64.2985          80.9730
92.8227          137.6341          169.1210
253.7666          274.1938          334.7916
367.2132          403.2170          406.9217
501.2125          513.6878          599.6726
621.7012          690.9846          701.7266
726.5832          798.5075          841.0485
860.3888          861.3892          876.9308

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892.5450	914.6193	961.4144
1006.4999	1033.1307	1055.6698
1085.1389	1136.2847	1138.3117
1159.5227	1188.7131	1190.8864
1243.2008	1268.6561	1291.8727
1303.4797	1319.8636	1336.8066
1354.8433	1375.3628	1391.1195
1410.3524	1416.1920	1475.0189
1477.8757	1484.9086	1486.3281
1504.2624	1560.5654	1688.4103
2960.6087	2973.7158	2987.3782
3008.2911	3035.1397	3047.2070
3066.0145	3069.3964	3073.5317
3087.6278	3092.6362	3147.6295
3164.0849	3254.2060	3261.2606

ZeroEnergy[kcal/mol] 27.49

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R4_ts5-----

Barrier R4_ts5 R4 R4-5

RRHO

Geometry[angstrom] 25

C	-0.9073169938	0.1232403437	2.3394438775
C	0.0783389827	-1.0850637732	2.4986851916
C	1.1158853428	-0.8312988346	1.4269859761
C	-0.31175718	-1.0264429838	-0.2674873225
C	-0.5613555776	0.3434431486	-0.1654778631
C	-0.3145888079	0.968213371	1.1779534374
C	1.2178044654	0.6707187746	1.3307451719
C	0.0464406477	-1.3853362375	-1.7003474976
C	-0.3107663163	1.039981978	-1.482217945
C	0.4226731036	-0.0260677282	-2.3371235701
H	-0.9425207595	0.716897728	3.2562094472
H	-1.9275711367	-0.1974999574	2.1199043604
H	-0.4178638734	-2.0549610203	2.4014676178
H	0.5412146342	-1.0749402185	3.4952535047
H	1.9712147343	-1.487365366	1.3024183173
H	-0.7984519388	-1.7769561042	0.3428976078
H	-0.5799071588	2.0255432407	1.2352252521
H	1.8111905667	1.0333944936	0.4891976186
H	1.6205855882	1.1177419535	2.2514462577
H	-0.8188334032	-1.8371491434	-2.2045433629
H	0.8578830784	-2.1161850032	-1.7633497977
H	0.2676479238	1.9651029883	-1.3772302584
H	-1.2650014763	1.3273106897	-1.9469351531
H	0.1668164187	0.0296510926	-3.3975758984
H	1.5026801359	0.1283495677	-2.2554169694

Core RigidRotor

SymmetryFactor 1.0

End

```

Tunneling      Eckart
ImaginaryFrequency[1/cm]  568.3231
WellDepth[kcal/mol]  32.51
WellDepth[kcal/mol]  24.38
End
Frequencies[1/cm]  68
104.6459          148.1565
209.4466          251.3457          269.7929
357.4859          418.9537          528.6434
603.6020          633.6803          662.0671
711.6773          764.5875          803.7182
820.5264          841.4852          859.7447
877.4279          887.2568          899.3206
909.2000          920.0528          958.8158
975.0469          982.3084          1024.1923
1030.7472         1041.9716          1052.7676
1106.9098         1133.2102          1156.6710
1164.2653         1179.6551          1204.3894
1230.6879         1241.4717          1245.7438
1272.5775         1280.9341          1304.2263
1315.8905         1324.8883          1326.2434
1337.7463         1374.2865          1461.1162
1482.1008         1486.6613          1488.3796
1491.2982         1506.6301          1511.5058
2975.2472         2982.2958          2985.7303
2993.2076         3023.0890          3038.5644
3046.2835         3048.5618          3055.5783
3077.6226         3082.7255          3084.2973
3091.1450         3161.4281          3163.1370
ZeroEnergy[kcal/mol]  32.51
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R4-5_ts1-----
Barrier      R4-5_ts1  R4-5  R4-5_i1
RRHO
Geometry[angstrom]  25
C  -0.66002645  1.3865684674  1.6438609067
C  -1.6045150134  -0.5387673209  2.3154366537
C  -0.4875736176  -0.7901570469  3.0645380962
C  0.648353599  -1.1053329601  -0.4970003504
C  0.715868314  0.1523650445  -0.0491537448
C  0.6482310269  0.6615468241  1.3729201827
C  0.8525812337  -0.4387860745  2.4759028887
C  0.7142861787  -1.1949083409  -2.0035283051
C  0.8407634432  1.1264766189  -1.2106202507
C  1.1889422853  0.2210860491  -2.4155457589
H  -0.7136086637  1.9970777298  2.5396486697
H  -1.2456028102  1.7514186305  0.8068442963
H  -1.6115230774  -0.6904047369  1.2422518187
H  -2.5869930091  -0.5249259721  2.7788248402

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H -0.5698443551 -0.9061584699 4.1407867748
H 0.5208415882 -1.9825305386 0.1269786088
H 1.4704425468 1.3856978338 1.4787879705
H 1.3926153283 -1.295443401 2.0602931103
H 1.4936800783 -0.0417748271 3.2699357084
H -0.2746842137 -1.4293121214 -2.4206978676
H 1.3895834008 -1.9815414559 -2.3553579322
H 1.5997963621 1.8947071545 -1.0268885841
H -0.1050633861 1.6617864907 -1.36659194
H 0.7411207177 0.565074411 -3.3501704553
H 2.2730044932 0.2103720119 -2.5585543365
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 583.7788
WellDepth[kcal/mol] 36.09
WellDepth[kcal/mol] 16.97
End
Frequencies[1/cm] 68
53.2459 78.8303
120.9616 167.6400 230.9138
272.8023 308.6810 367.5968
453.6098 508.2856 551.6091
608.3867 630.9662 650.5097
707.5831 778.2517 814.8764
833.6569 856.1069 882.7116
902.9512 907.0095 915.0246
917.3412 934.1397 952.6862
974.6176 1010.1369 1040.7620
1056.9524 1068.7487 1095.1797
1144.7211 1160.7867 1194.0661
1222.4689 1229.5943 1240.3880
1270.0479 1283.8149 1313.3666
1326.6868 1328.0847 1344.9084
1375.0830 1424.5458 1457.8846
1485.0364 1485.7073 1490.5871
1509.8515 1561.6392 1699.0080
2959.4584 2991.8922 2999.8866
3028.0570 3030.6735 3039.0362
3050.2424 3051.8846 3088.0744
3115.3607 3119.6148 3150.9570
3179.1301 3195.8145 3208.6562
ZeroEnergy[kcal/mol] 44.22
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-5_ts2-----
Barrier R4-5_ts2 R4-5_i1 R4-5_p1
RRHO
Geometry[angstrom] 25

```

C	-1.125317196	1.3275557606	1.05253304
C	-0.3772265576	-1.7708495889	2.9657801236
C	0.5755180738	-1.4178221175	2.0797316744
C	-0.6154237067	-0.6646207789	-1.2472711417
C	0.2725138952	0.174620258	-0.6981497468
C	0.1131372439	1.0257052018	0.5002691316
C	1.1542717878	-0.106800275	1.9759772032
C	-0.0981050429	-1.3202209528	-2.5039707528
C	1.5515081773	0.2127827943	-1.5183944799
C	1.4179204085	-1.0004179292	-2.468689968
H	-1.2223983182	2.1103599687	1.7950510652
H	-2.0041806541	0.7281589524	0.8514202094
H	-0.746615107	-1.0708828069	3.7086325637
H	-0.8020802987	-2.7675566859	2.975753193
H	0.9019702997	-2.1556383555	1.3511794544
H	-1.6189267106	-0.8364157762	-0.8759677265
H	0.8726863973	1.7982185895	0.5972656158
H	2.130146246	-0.0243817201	1.5090553083
H	1.0008870254	0.5738325853	2.8068723193
H	-0.5833179727	-0.890257451	-3.3914677258
H	-0.2970762108	-2.3964390932	-2.5389175579
H	2.4540327841	0.1618286077	-0.9002062756
H	1.6098159373	1.1598602018	-2.071753575
H	1.8355804255	-0.811432341	-3.4596893605
H	1.9573240737	-1.8529360478	-2.0464295915

Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 600.7223
WellDepth[kcal/mol] 7.41
WellDepth[kcal/mol] 5.26
End
Frequencies[1/cm] 68

28.9026	47.9045	
99.9883	103.9816	152.5809
213.4492	225.2837	243.1498
333.0968	406.3974	427.3744
445.6196	545.6283	598.2025
643.9791	670.3103	746.5137
756.3467	816.3882	826.6250
853.4298	881.5803	891.0888
905.9719	916.1241	957.9198
961.7883	1001.7808	1019.1686
1026.1508	1060.3005	1062.0131
1069.9311	1137.6634	1156.6423
1214.0678	1228.2528	1232.9397
1256.6857	1282.3399	1316.2969
1318.4482	1326.9749	1347.3504
1433.5731	1436.8348	1485.4544
1488.8109	1494.5503	1511.4736
1518.5098	1613.4227	1683.4410

```

2987.2182          2995.8614          3030.0948
3038.0293          3051.3981          3088.0358
3113.9982          3120.3602          3129.3434
3138.9714          3143.2263          3182.8799
3202.8228          3218.0736          3233.8168
ZeroEnergy[kcal/mol] 34.66
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-5_ts3-----
Barrier          R4-5_ts3  R4-5_i1  R4-5_p2
RRHO
Geometry[angstrom] 25
C -0.0973534237    1.9929900547    1.3064783482
C 0.9089227061    -1.3520696883    -0.8649902147
C 0.8677918605    -0.046075747    -0.6561060552
C 0.8588536987    1.043916761    1.4510548043
C 0.8303628345    -1.6468385402    -2.3590146173
C 0.7429289441    0.7929482037    -1.8922893849
C 1.0419483313    -0.2508776206    -3.0122713113
H 0.1018233273    2.9110577274    0.7664108367
H -1.1050689955    1.8412021193    1.6759966866
H 0.9494470753    -2.1337109908    -0.1154084207
H 1.8796927732    1.289969459    1.1743701163
H -0.1508222023    -2.0695005693    -2.6112267002
H 1.579907506    -2.3738641743    -2.6872751862
H 1.4356760454    1.6391612032    -1.9155982984
H -0.2684845908    1.2093152773    -1.9721400805
H 0.4212041541    -0.1022976472    -3.8983311363
H 2.0851426775    -0.1518500034    -3.3225678455
C -1.3709870013    -0.805531109    3.6073368937
C -0.6881455299    -0.7002290187    2.471139012
C 0.7131254217    -0.1702570192    2.3507591985
H -0.947829022    -0.4946551034    4.5581456462
H -2.3767524381    -1.2103435512    3.6306903762
H -1.150336178    -1.0146067341    1.5378602915
H 1.3713669031    -0.9620228426    1.9764663744
H 1.0935061226    0.0936375538    3.3458056666
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 269.1961
WellDepth[kcal/mol] 38.24
WellDepth[kcal/mol] 1.68
End
Frequencies[1/cm] 68
20.6283          47.1844
70.8274          96.7734          111.4501
141.7661         180.2735          233.0988
265.8077         389.3664          420.8796

```

490.5134	535.7283	616.5506
674.6908	722.5968	767.8241
812.9898	872.5638	875.1617
885.6561	890.4551	912.9785
930.9364	946.2468	948.2663
961.0707	994.8173	1019.5525
1042.4470	1050.7869	1082.0120
1132.4888	1136.0161	1195.6077
1217.6606	1237.8979	1246.0841
1291.8451	1297.5238	1305.6312
1317.5981	1335.1448	1341.7057
1431.4510	1452.8323	1478.6220
1481.6587	1488.6276	1505.2152
1581.0352	1656.5045	1707.2970
3000.2515	3009.2265	3013.7919
3038.5255	3042.1584	3049.0225
3057.2870	3092.0183	3122.1585
3134.8786	3137.4201	3146.6717
3177.5759	3206.2424	3224.5000
ZeroEnergy[kcal/mol] 65.49		
ElectronicLevels[1/cm] 1		
0 2		
End		
!-----		
End		

R4_seconadary_c8h11_3

```
!-----c10h15_R4-1_rpl-----
Well          R4-1_rpl
Species
RRHO
Geometry[angstrom]  19
C  -0.7480168784   0.4461380072   1.5652472949
C  -0.2963109615  -1.0466439883   1.6492103454
C   0.6468078167  -1.1927671543   0.4057072171
C  -0.2219321609  -1.0590271797  -0.8201137362
C  -0.6383465515   0.2783330786  -0.9072004212
C  -0.0012667485   0.9713714605   0.2989403671
C   1.3325302795   0.1977758744   0.4085790584
C  -1.4774444143   0.8607988651  -1.8238023616
H  -0.4328906671   1.0042680385   2.450817577
H  -1.829606348   0.5561388334   1.4707765973
H  -1.1330267929  -1.746140816   1.6093251728
H   0.2595010194  -1.2452621363   2.5702359847
H   1.2943844668  -2.068879875   0.4387352466
H  -0.5604383355  -1.8746244119  -1.4469222903
H   0.0553953996   2.0576676896   0.2270901558
H   1.9889229298   0.3503671648  -0.4505007316
H   1.8808139087   0.4080342735   1.3319840198
H  -1.7333411179   1.9120804163  -1.7688290407
H  -1.901381844   0.2860978594  -2.6395404552
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
160.7614           249.4086           344.8050
388.0216           455.1904           541.0703
556.5269           623.9510           686.4251
725.1989           783.4013           798.5429
820.1372           836.7626           873.3434
881.6202           921.5896           938.1474
952.2232           963.6577           989.7240
1036.0866          1049.3634          1129.9936
1134.8773          1166.4914          1191.8440
1238.3811          1250.6178          1280.5289
1285.3558          1294.9792          1315.7410
1332.4062          1360.1192          1419.6271
1492.5268          1494.6820          1515.9188
1523.5593          3035.5863          3038.1308
3050.8281          3082.0073          3094.6958
3097.5385          3101.0784          3101.7777
3134.9457          3193.3579          3224.1973
ZeroEnergy[kcal/mol] 25.1
ElectronicLevels[1/cm]  1
0  2
End
```

```

End
!-----
!-----c10h15_R4-1_ip2-----
Well      R4-1_ip2
Species
RRHO
Geometry[angstrom]  19
C  -0.7638943413    0.4542340522    1.5615559426
C  -0.3218236209   -1.013070333    1.6428854353
C   0.35809481    -1.4574527417    0.3771660074
C   0.8629802417   -0.5989933413   -0.5202464769
C   0.8383145847    0.8532986734   -0.3426102345
C   0.365538939    1.3587526051    1.0163644212
C   1.5036188515    1.4741260466    1.9828840679
C   1.2401883015    1.6912809552   -1.3075371667
H  -1.084056004    0.8135282637    2.5444805911
H  -1.6276476517    0.532454177    0.8930462981
H  -1.1855757     -1.6558499618    1.8457318862
H   0.3615735046   -1.1555191232    2.4916880244
H   0.4331257961   -2.5258016493    0.1952363267
H   1.3179016893   -0.9760132341   -1.4321329142
H  -0.063111289    2.3639322558    0.8644968195
H   2.516740312    1.6285252906    1.6347563207
H   1.3078308582    1.5438706447    3.0477960403
H   1.2140766901    2.7672848657   -1.1742920284
H   1.6097020282    1.3226145546   -2.2586743608
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
94.1741            99.4413            197.0424
235.7360           337.8043            359.6858
394.9334           470.8706            474.8896
591.6856           621.5494            706.6993
721.8704           777.8913            814.8276
852.5552           895.8754            909.7455
953.2185           969.7250            987.9704
1001.3367          1024.2526           1090.1045
1110.5608          1166.7431           1190.8894
1238.2926          1277.2885           1307.0074
1332.1292          1369.3073           1372.1536
1405.8680          1448.3858           1460.0374
1474.1240          1495.3264           1658.8448
1696.8074          2924.0474           2992.2996
3024.6703          3039.6507           3065.4580
3126.8473          3128.4910           3136.8315
3158.7479          3210.3522           3237.6898
ZeroEnergy[kcal/mol]  38.72
ElectronicLevels[1/cm]  1
0  2
End
End

```

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!-----
!-----c10h15_R4-1_ip3-----
Well      R4-1_ip3
Species
RRHO
Geometry[angstrom]  19
C  -0.8106419396    0.4369763874    1.4821082208
C  -0.316693874    -1.007793268    1.6485422543
C   0.3203293896    -1.5156226618    0.383282351
C   0.8897188202    -0.6805065948    -0.490043585
C   0.9487783639    0.7831681387    -0.2845700961
C   0.1665469381    1.3299522508    0.7601618292
C   0.1156014634    2.7966395361    1.061385001
C   1.7535276504    1.5274023565    -1.1246196802
H  -1.0619749928    0.8641722927    2.4580528085
H  -1.7540937229    0.4199683924    0.9099573795
H  -1.1476398836    -1.6535264491    1.9487550321
H   0.4180812864    -1.0596701085    2.4653050499
H   0.3457687343    -2.5872232604    0.2106861327
H   1.3709063247    -1.068994253    -1.3824116649
H  -0.719978887    3.2847129407    0.5374335136
H   1.0283002447    3.3191402959    0.770942068
H  -0.0436162345    2.9687988592    2.1303445364
H   1.8468031185    2.6014660387    -1.0439204055
H   2.3287552    1.0433331066    -1.9043337454
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
24.4077          107.4010          144.1309
285.1865          344.7111          366.6883
402.8893          473.9247          499.7425
581.2033          597.4055          697.4323
710.9768          765.7046          797.7749
855.8938          891.8605          949.7333
973.4554          986.4724          995.6155
1046.4298         1049.9669          1157.5557
1184.3668         1187.7912          1234.8992
1271.0067         1322.0858          1335.0169
1381.2785         1406.3542          1416.3488
1436.2371         1468.5986          1481.5676
1485.8492         1496.6653          1527.4901
1693.5503         2935.4725          2976.0582
2982.4577         3044.2181          3049.6166
3050.9670         3103.9329          3143.9974
3153.3384         3166.9468          3242.3101
ZeroEnergy[kcal/mol]  25.1
ElectronicLevels[1/cm]  1
0  2
End
End
!-----

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!-----c10h15_R4-1_ip4-----
Well          R4-1_ip4
Species
RRHO
Geometry[angstrom]  19
C  -0.9482257482    0.3623242316    1.4348967739
C  -0.3604897525   -0.9957034085    1.6140616464
C   0.4501895171   -1.4399404439    0.4280039256
C   0.6680212643   -0.6614790598   -0.6387789755
C   0.1982911974    0.7232215269   -0.7483736565
C  -0.2770934055    1.3732424365    0.5539886405
C  -1.1360818999    2.6298714939    0.3692895273
C   0.2393322833    1.3629423791   -1.9249230594
H  -1.7320837382    0.6917110046    2.1084973203
H  -1.1518405634   -1.7319139741    1.8137974571
H   0.2764703396   -1.0326864206    2.5193905149
H   0.8416383246   -2.4527947526    0.4463939893
H   1.2165077116   -1.0583797976   -1.4885931738
H   0.6547630636    1.6897325575    1.0656215304
H  -2.0425064613    2.4031340369   -0.1982104709
H  -0.5928938229    3.4204884642   -0.1522842998
H  -1.4338896383    3.0251285773    1.344149036
H  -0.1031391869    2.3814017843   -2.0515268507
H   0.6224215155    0.8663313644   -2.8102788752
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
73.8182           138.3185           242.1777
289.0234           330.3087           343.8173
394.1192           451.9900           463.8640
534.4101           597.1509           675.5203
753.1592           797.2899           823.0850
877.3540           907.2883           907.7988
939.3103           979.0603           998.2326
1022.4202          1075.5045          1105.8985
1148.2887          1178.6370          1193.7172
1269.6628          1286.2694          1305.6949
1358.3400          1389.9343          1404.7852
1410.6244          1449.4224          1457.4673
1497.3470          1511.0856          1661.1505
1699.6229          2861.4772          2888.1823
2991.8711          3031.2369          3092.8999
3102.9977          3136.9836          3140.9999
3160.8564          3163.4050          3226.4023
ZeroEnergy[kcal/mol] 36.81
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----c10h15_R4-1_ip5-----

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Well          R4-1_ip5
Species
RRHO
Geometry[angstrom]  19
C  -0.2136953771    0.0035461075    1.6847181526
C  0.2203570022   -1.4353015702    1.6952957276
C  0.979506746   -1.8264299751    0.4605890378
C  1.1490708703   -1.0112339687   -0.5775510606
C  0.5506437154    0.3818286657   -0.6658211841
C  -0.0620555638    0.835922838    0.6527732557
C  -0.4869179539    2.2795337303    0.7146783869
C  -0.45977473    0.4016751247   -1.7813577001
H  -0.6695173954    0.3770523016    2.5990457107
H  -0.653354715   -2.0931582106    1.8211375988
H  0.8378830447   -1.6276445461    2.5848041789
H  1.4137983534   -2.8224162982    0.4393124182
H  1.7116454846   -1.3426473726   -1.4455079699
H  1.3544341665    1.0849414065   -0.9289144369
H  -1.2146494718    2.5121234792   -0.0699224408
H  0.3704747858    2.9448406702    0.5556957821
H  -0.9321706504    2.5252341193    1.6809445279
H  -0.2013772947    0.7494385148   -2.7743354008
H  -1.410773017   -0.0989050164   -1.6403485841
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
78.1081          125.5635          173.2572
228.3285          249.9773          289.4488
347.0197          446.4373          479.5557
542.5970          561.5182          590.9537
710.2358          734.8144          823.6394
845.6140          897.1339          949.3430
984.1155          1004.1016         1020.9249
1031.9421          1061.8422          1091.2094
1095.9924          1164.5769          1205.3334
1218.3328          1299.3317          1324.6978
1365.1930          1376.3946          1411.0658
1415.5439          1450.2360          1472.0257
1477.6991          1495.2011          1700.7037
1745.9881          2971.8046          2974.2973
2984.7839          3008.3589          3053.6466
3098.9933          3128.6186          3129.3264
3133.5262          3158.1614          3238.8495
ZeroEnergy[kcal/mol]  39.91
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----c10h15_R4-1_ip6-----
Well          R4-1_ip6

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Species
RRHO
Geometry[angstrom] 19
C -0.1821411047 0.0380644342 1.7053665319
C 0.2379048873 -1.3977879591 1.7946196344
C 0.8589531215 -1.9048345995 0.530138424
C 1.0052241544 -1.1046593954 -0.5619302737
C 0.5873765284 0.2527497029 -0.5891520846
C -0.0177479242 0.8069781019 0.5906510247
C -0.4722129987 2.2482987124 0.5915339716
C 0.7799206266 1.0790520825 -1.8302797374
H -0.6415327999 0.4740176659 2.5876715118
H -0.6264491816 -2.0279690496 2.0732178233
H 0.9338174706 -1.5360872324 2.6422385081
H 1.1941767455 -2.9361715488 0.5020344873
H 1.4617363436 -1.5153748156 -1.4585404794
H -1.223352284 2.4336544585 -0.1832517578
H 0.3601539663 2.932441651 0.3965882936
H -0.9098317597 2.5187959113 1.5539745957
H 1.4121379953 1.9568959116 -1.6482262644
H -0.1703626882 1.4592012911 -2.2250945096
H 1.2525299014 0.4920226771 -2.6202896995
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 51
103.1773 125.0061 176.1457
241.6721 265.4374 300.9173
402.5094 425.4106 482.5579
564.1131 596.0970 707.2474
711.0575 767.6704 798.9528
906.7914 937.5391 956.8584
975.3781 989.7654 1028.4026
1060.5928 1073.9012 1155.7565
1180.9323 1184.6951 1240.1833
1265.5854 1322.4255 1382.7814
1413.0145 1423.3469 1442.5916
1453.4479 1476.2429 1486.0250
1493.0741 1502.1372 1542.1376
1620.7352 2895.4228 2913.3096
2997.5578 3020.4539 3030.7776
3065.2541 3095.1227 3103.7094
3139.8167 3148.1569 3167.8402
ZeroEnergy[kcal/mol] 14.82
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R4-1_ip7-----
Well R4-1_ip7
Species

```

```

RRHO
Geometry[angstrom] 19
C -0.2666197097 0.004341737 1.6744008451
C 0.1684463086 -1.4248309463 1.7570087124
C 0.8124454304 -2.0253153183 0.7212645455
C 1.094890832 -1.3194767688 -0.4736418484
C 0.7183216794 0.0398747893 -0.6383686038
C 0.0634219713 0.6999987249 0.3769378861
C -0.3752663585 2.1334453279 0.299945578
C 1.0583321542 0.7225093578 -1.9489439137
H -1.3549724324 0.078137093 1.85943557
H 0.1661489978 0.5791191346 2.5149590257
H -0.0452653007 -1.9704694478 2.6699800763
H 1.1186946288 -3.0634524574 0.8038719606
H 1.6097713217 -1.8251898249 -1.2822312879
H -1.46126375 2.2176335598 0.4401344712
H -0.124291337 2.6089443092 -0.6474535535
H 0.0820191963 2.7256129293 1.103924404
H 1.7117399349 1.5875095563 -1.8004243633
H 0.1627841976 1.0765912787 -2.4684172515
H 1.5747282356 0.0326369656 -2.6187012529
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 51
93.4042 103.6373 135.4354
177.5808 295.9037 315.9915
387.2156 469.3986 499.6026
537.3411 568.7706 670.4440
711.9292 772.5405 810.1663
907.3532 920.0276 965.2164
976.3903 1009.0249 1030.8529
1057.3591 1091.2841 1149.9745
1177.1077 1190.6137 1194.8114
1265.5374 1312.2991 1402.1838
1412.3496 1417.6450 1432.3999
1439.4977 1478.3300 1482.3689
1499.0038 1503.8286 1561.4402
1607.8892 2885.2592 2903.3110
2990.9868 3020.4327 3024.9960
3073.3579 3101.8399 3122.0348
3149.2780 3168.0365 3180.1988
ZeroEnergy[kcal/mol] 14.82
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R4-1_ip8-----
Well R4-1_ip8
Species
RRHO

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Geometry[angstrom] 19
C -0.1288714679 0.0533374312 1.7360951637
C 0.2170917034 -1.2623428464 1.7891545254
C 0.7696848589 -1.9164048206 0.6614839958
C 0.9919491294 -1.1849680436 -0.5284298646
C 0.6661168781 0.1379849275 -0.6537665561
C 0.0076156126 0.8850108508 0.4892090326
C -1.3740948209 1.4774331821 0.0883582708
C 0.9634529213 0.9069683001 -1.9091065587
H -0.5463315147 0.5451021284 2.6095819808
H 0.0753136956 -1.8191858247 2.7100423588
H 1.0404619831 -2.9636477261 0.7140550087
H 1.4533441218 -1.6910781363 -1.3721288325
H 0.6432119696 1.7594109521 0.7241017099
H -2.057436302 0.6795560784 -0.2126055026
H -1.2816243897 2.1877360856 -0.7362983586
H -1.8182095661 2.0052033389 0.9366175188
H 1.5312623208 1.8197284756 -1.6874491626
H 0.0499207198 1.2273923283 -2.4236407563
H 1.546566147 0.3084193185 -2.6119819733
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 51
67.5355 150.7695 212.0023
234.8298 291.1234 356.9406
396.5251 485.4409 492.4559
573.0282 624.9406 677.6750
733.0516 773.6725 831.2166
909.0086 937.7077 966.4034
980.2960 1013.4979 1025.5263
1047.1420 1061.8849 1101.2243
1133.2111 1178.6000 1196.4006
1283.5217 1307.2395 1337.4686
1391.8941 1412.5742 1414.8584
1430.0910 1475.4540 1487.7467
1500.4862 1502.4466 1544.3784
1610.1759 2890.2088 2998.5111
3027.9874 3037.4412 3094.4570
3095.8474 3104.7539 3142.5508
3145.5583 3164.6138 3191.4403
ZeroEnergy[kcal/mol] 15.54
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R4-1_ip10-----
Well R4-1_ip10
Species
RRHO
Geometry[angstrom] 19

```

```

C  -1.2573369094    5.084711E-4    2.3366638132
C  -0.7025175799   -1.0295964119    1.4057514888
C  -0.7497964631   -0.6129868813   -0.0411848711
C   0.2812457078   -0.3395390281   -0.8482818435
C   1.7235031992   -0.3476964361   -0.508664647
C   2.638642697   -1.0961529102   -1.3839802121
C   2.2796906231   -1.9112249654   -2.3799305653
C   2.2160310568    0.3442184089    0.5339507179
H  -1.6544532065   -0.2844710502    3.303354227
H  -1.1772583682    1.0556800157    2.1064214182
H  -1.2738437038   -1.9608627969    1.5230802163
H   0.3320709558   -1.2801643642    1.6845017515
H  -1.7496630236   -0.5382982003   -0.4635847819
H   0.0579041048   -0.1024244482   -1.8864099024
H   3.6967133332   -0.9588129353   -1.1725217256
H   1.2401183355   -2.0994052174   -2.6232277639
H   3.0228524275   -2.425548129   -2.9775966392
H   3.2780717469    0.3397438453    0.7558705294
H   1.579593067    0.9376150335    1.1780667896
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 51
44.5691          74.4282          112.5855
152.5631         172.2793         212.9425
305.8019         369.5965         399.4655
468.2111         504.6411         568.7637
588.6404         696.9507         781.5550
792.5387         816.7783         834.0689
928.8341         941.9958         944.3653
1006.2014        1014.9806        1029.2965
1052.7944        1063.6078        1090.4972
1199.4500        1278.8811        1293.7513
1326.6428        1335.2039        1418.1521
1439.4140        1458.1269        1462.9562
1463.9344        1645.5922        1688.5466
1701.2116        2965.9183        2999.8513
3117.5256        3131.0447        3135.4461
3137.6256        3140.3393        3144.3458
3224.2000        3227.2995        3241.2938
ZeroEnergy[kcal/mol] 60.23
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----h_c8h10_R4-1_p9-----
Bimolecular R4-1_p9
Fragment c8h10
RRHO
Geometry[angstrom] 18
C 0.0181397273 0.3685073464 1.6340610929

```

```

C 0.4151914921 -0.9645173907 1.7103422342
C 1.0159315495 -1.5644058789 0.6093494501
C 1.2120056612 -0.8236549961 -0.5539507421
C 0.8183211588 0.513714157 -0.642995718
C 0.2092104712 1.1219643523 0.4733433528
C -0.2330810041 2.5645632582 0.4251415184
C 1.0461335303 1.2871829275 -1.9192741908
H -0.4509138645 0.836853153 2.4937180996
H 0.2551934819 -1.5269581108 2.6235013682
H 1.3308888596 -2.601120431 0.6520600262
H 1.6810429854 -1.292079843 -1.4135741239
H -0.9723329099 2.734826087 -0.3648290037
H 0.6062966368 3.2384136754 0.2228478214
H -0.6824558439 2.8678432985 1.372382765
H 1.6855826872 2.1608902292 -1.75403426
H 0.1058934766 1.6589640463 -2.3402869965
H 1.5251839045 0.6624121196 -2.6751546938
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 48
132.3421 163.4797 174.7376
257.7441 299.7971 411.4220
448.3007 511.1731 521.7517
591.0939 729.4119 746.0974
755.7121 836.0310 877.0097
943.8281 989.2073 1003.9809
1011.5689 1045.8229 1071.4634
1074.0342 1143.4258 1184.5922
1203.8783 1242.6632 1316.3627
1326.3758 1414.4027 1424.8946
1467.9850 1481.4736 1496.0720
1496.6132 1504.3487 1523.9641
1620.2671 1649.6777 3017.1697
3017.7611 3059.5807 3061.4834
3101.6567 3103.0901 3151.7026
3156.3045 3170.1746 3185.1908
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 33.94
End
!-----ch3_c7h8_R4-1_p14-----
Bimolecular R4-1_p14
Fragment c7h8

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RRHO
Geometry[angstrom] 15
C -1.5859253695 0.3603087539 0.6031861375
C -0.3170806041 0.0316385649 1.0746822957
C 0.7733581132 -0.0634901389 0.2037435599
C 0.5546998392 0.1751408462 -1.1570959493
C -0.7121130138 0.5041455052 -1.6337938534
C -1.788343386 0.5989274878 -0.7543188476
C 2.154062483 -0.3886604541 0.7221680017
H -2.4175241098 0.4261346268 1.2963227141
H -0.1706849106 -0.1561239174 2.1338552086
H 2.6973119257 0.5234725223 0.9930227207
H 1.3859872864 0.1001172192 -1.8512618829
H -0.8590336601 0.6826750629 -2.6934491487
H -2.7757242043 0.8519566561 -1.1237413162
H 2.7495900587 -0.9116551661 -0.0297820897
H 2.1073245508 -1.017377569 1.6144324525
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 39
25.2791 208.3916 343.7877
415.2520 476.5453 529.2377
637.7431 713.6407 744.5489
798.9305 855.0919 910.5769
975.7862 999.1745 1000.8220
1017.9113 1051.4699 1062.6347
1111.5615 1180.9829 1203.1449
1228.9765 1327.9160 1355.9448
1414.7593 1470.4004 1491.3629
1503.9825 1529.6569 1626.8235
1648.8606 3020.1450 3074.4788
3100.6412 3150.9983 3152.6365
3165.2227 3173.5642 3186.3301
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment ch3
RRHO
Geometry[angstrom] 4
C 0.0 1.995E-7 0.0
H 0.0 1.0804553795 0.0
H 0.9357017515 -0.5402277895 0.0
H -0.9357017515 -0.5402277895 0.0
Core RigidRotor
SymmetryFactor 6
End
Frequencies[1/cm] 6
505.1501 1403.0831 1403.0885
3103.6402 3282.6573 3282.6683
ZeroEnergy[kcal/mol] 0.0

```

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ElectronicLevels[1/cm]      1
0  2
End
GroundEnergy[kcal/mol] 25.10
End
!-----c2h4_c6h7_R4-1_p11-----
Bimolecular      R4-1_p11
Fragment          c6h7
RRHO
Geometry[angstrom]      13
C  -1.6342206836    0.3745969637    1.0301065855
C  -0.6684592972    0.4795520041    0.1490075986
C   0.7864649132    0.4243344877    0.4425933957
C   1.674212993    -0.2288658664   -0.5280224116
C   1.2979137387   -0.919787224   -1.6080859988
C   1.2912713298    0.9763528068    1.5590407324
H  -2.7138001123    0.3912803474    1.0350048309
H  -0.936983324    0.6212102457   -0.9038606085
H   2.7359575404   -0.1311446455   -0.3139880794
H   0.2561725338   -1.074573182   -1.8648812003
H   2.0316921394   -1.3677321321   -2.2673769997
H   2.352682154    0.9279702451    1.7755440519
H   0.6566590749    1.4862779495    2.2725791032
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]      33
102.3394              147.4103              246.2025
307.1517              397.4239              499.3510
529.5578              630.1924              721.8462
736.7550              779.8269              862.9489
893.4548              930.0291              937.1562
979.5734             1026.2951             1058.9940
1236.5748             1325.8423             1326.6601
1420.3003             1461.0189             1639.6876
1658.5517             1690.7905             3026.1566
3133.8388             3142.1244             3145.2063
3224.1420             3232.9226             3240.9830
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]      1
0  2
End
Fragment          c2h4
RRHO
Geometry[angstrom]      6
C   0.0    0.6634900906    0.0
C   0.0   -0.6634900906    0.0
H   0.0    1.23462754   -0.9225248038
H   0.0    1.23462754    0.9225248038
H   0.0   -1.23462754    0.9225248038
H   0.0   -1.23462754   -0.9225248038
Core RigidRotor

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SymmetryFactor 4
End
Frequencies[1/cm] 12
834.2929          972.9227          974.1218
1066.8559         1238.5875         1379.4650
1472.0483         1691.5384         3121.2072
3136.3255         3192.3844         3220.8390
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 93.21
End
!-----c10h15_R4-1_ts2-----
Barrier          R4-1_ts2  R4-1_rp1  R4-1_ip2
RRHO
Geometry[angstrom] 19
C -0.7433868794  0.4726531437  1.6054812313
C -0.1998583428  -0.9746140709  1.7128517448
C 0.4047310314  -1.3936512631  0.3802100049
C -0.2120906549  -1.0427110314  -0.8135476024
C -0.6872378797  0.325740262  -0.8738641871
C -0.1047025026  1.0650329661  0.327910699
C 1.3581552582  0.682659337  0.3783392598
C -1.4159713289  0.8887491124  -1.8521297045
H -0.4617558719  1.0583250108  2.4852188537
H -1.8328834683  0.4953546021  1.5319986152
H -1.0025276452  -1.6760447895  1.9692332629
H 0.5499188357  -1.0606504848  2.5032327311
H 1.0372540697  -2.2780707874  0.4039916421
H -0.100752113  -1.6367999434  -1.7142837755
H -0.2779565686  2.144950789  0.2535819571
H 1.9426082301  0.7380858843  -0.533735323
H 1.9093344929  0.849878001  1.3008717536
H -1.6530806207  1.9465661071  -1.8445718204
H -1.7885380421  0.304131155  -2.6864673428
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 581.011
WellDepth[kcal/mol] 35.37
WellDepth[kcal/mol] 21.75
End
Frequencies[1/cm] 50
145.3902          227.6383
335.4470          382.9939          393.9579
497.7222          549.1754          583.9513
644.3228          689.0485          746.2766
759.5076          792.7445          822.2326
854.8196          878.1223          892.5269
893.9539          948.8707          968.2967

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990.4780          1004.2789          1062.9660
1081.1724          1140.9697          1170.1926
1204.7642          1246.8262          1276.5152
1300.7375          1329.3823          1337.9644
1372.8742          1443.8000          1462.0895
1465.7843          1493.3070          1511.3096
1648.7438          3016.6362          3018.4968
3042.8173          3058.5134          3086.7817
3102.9427          3130.6881          3135.7435
3167.7736          3204.2822          3214.2461
ZeroEnergy[kcal/mol] 60.47
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-1_ts3-----
Barrier          R4-1_ts3  R4-1_ip2  R4-1_ip3
RRHO
Geometry[angstrom] 19
C 0.1306627749 -0.0103530801 2.0919161254
C -0.6416150688 -1.1416412832 1.3997401439
C -0.0035399087 -1.5265928832 0.0922108602
C 0.7902324755 -0.6909409334 -0.5880796692
C 1.1166081519 0.6731984037 -0.1475862673
C 0.5395636665 1.0869779774 1.1310035483
C 0.7184606568 2.4504610668 1.6845886663
C 1.8998072688 1.4670432374 -0.9213743407
H 1.045582591 -0.4204859948 2.5438340143
H -0.4602743331 0.4060841874 2.9133179991
H -1.6799713905 -0.8274341865 1.2185281451
H -0.7034658409 -2.0110178524 2.0626951944
H -0.2226445328 -2.510885633 -0.3102432103
H 1.226974095 -1.0093270572 -1.5300715213
H -0.3648837274 1.9580468731 1.0185616019
H 1.1772007153 3.233826537 1.1016247205
H 0.4736196676 2.6302295946 2.7214900256
H 2.1972345328 2.4635624655 -0.623631377
H 2.2650432061 1.1152145609 -1.8787676593
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 1815.4218
WellDepth[kcal/mol] 31.79
WellDepth[kcal/mol] 45.41
End
Frequencies[1/cm] 50
103.0768          181.1818
295.7098          329.8637          381.8427
395.8515          430.1478          472.5153
512.0439          601.2940          651.8560
666.4478          718.5351          734.0867

```

788.9170	829.5165	856.7002
886.8110	947.3486	972.3723
992.6152	1030.5524	1046.0767
1162.0851	1179.4403	1189.6712
1236.7534	1247.7914	1277.9532
1343.3623	1359.4336	1391.2794
1422.0996	1438.9516	1456.0106
1477.4819	1487.1271	1592.8257
1691.8729	2174.1154	2974.9241
2985.4133	3042.7939	3052.6055
3142.3910	3149.5134	3165.0062
3168.4214	3232.8557	3283.9756

ZeroEnergy[kcal/mol] 70.51

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R4-1_ts4-----

Barrier R4-1_ts4 R4-1_ip3 R4-1_ip4

RRHO

Geometry[angstrom] 19

C	-0.5005301196	0.3932514581	1.7086917939
C	-0.5942979131	-1.0717975218	1.3989777586
C	0.4562504754	-1.5181893682	0.4147350387
C	1.1771322102	-0.6740640342	-0.3306135184
C	1.0524976973	0.7918847026	-0.2704370305
C	0.2863266869	1.3343773709	0.8440055993
C	-0.0394467417	2.8022596674	0.9309097923
C	1.6388779679	1.5538431704	-1.2284310167
H	0.7523622906	0.8823871171	1.9275177199
H	-1.1765536124	0.8440819199	2.4235509253
H	-1.5906256644	-1.3085137909	0.9808038743
H	-0.5288477595	-1.6718592855	2.3160223986
H	0.5900855145	-2.5889351218	0.2927598988
H	1.8888281679	-1.0694941903	-1.0490702095
H	-0.8190136319	3.0682108117	0.2054062201
H	0.8323182477	3.428468247	0.7292401477
H	-0.4136604392	3.0615827494	1.9246818435
H	1.5523036333	2.6317913653	-1.2521041717
H	2.2139359901	1.0913107326	-2.0214600641

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1877.0239

WellDepth[kcal/mol] 44.93

WellDepth[kcal/mol] 33.22

End

Frequencies[1/cm] 50

98.2970	166.7636	
195.3717	280.6609	329.6866
374.0248	406.4400	475.2036

515.9594	602.8604	612.1273
672.3492	704.3622	777.2930
812.5126	828.9509	890.3741
929.7679	969.4656	991.7435
1000.0394	1037.3340	1074.7448
1137.1216	1179.3314	1195.4707
1235.7739	1247.2431	1333.8303
1362.8458	1397.6977	1412.5590
1423.2380	1451.2914	1477.8075
1488.7662	1504.4506	1598.2720
1700.9822	2150.9525	2893.7338
2995.0368	2999.9702	3066.2568
3096.4321	3142.7191	3150.5470
3164.8141	3187.5578	3235.2630

ZeroEnergy[kcal/mol] 70.03

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R4-1_ts5-----

Barrier R4-1_ts5 R4-1_ip4 R4-1_ip5

RRHO

Geometry[angstrom] 19

C	-0.8570940309	0.3880286956	1.5086285366
C	-0.3380434144	-1.0153304246	1.6378395685
C	0.388946399	-1.4797686837	0.4032376486
C	0.6487834501	-0.6937762797	-0.6425942653
C	0.2028946741	0.7162772651	-0.7371682817
C	-0.5609009528	1.2231758422	0.4460703315
C	-1.2021924192	2.5850513804	0.3348749028
C	0.2867539636	1.3735841366	-1.959105369
H	-1.4262552936	0.7948095482	2.3373407322
H	-1.1595574484	-1.710709385	1.8696923045
H	0.3379330813	-1.099927743	2.5068081885
H	0.7245045055	-2.5128431791	0.3880186733
H	1.1865779657	-1.0839492744	-1.5003606141
H	0.8296020507	1.3987083638	0.2770148822
H	-2.0253826638	2.554670137	-0.387536883
H	-0.496516268	3.3454601944	-0.0101475326
H	-1.6001890067	2.9040432257	1.2992454744
H	-0.1261537576	2.3588049318	-2.1216641662
H	0.8547511654	0.9297052486	-2.7657691313

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1734.8337

WellDepth[kcal/mol] 38.95

WellDepth[kcal/mol] 35.85

End

Frequencies[1/cm] 50

101.1110	203.6664
----------	----------

216.7575	297.5730	322.3359
394.4791	427.5828	483.3138
547.0616	552.4638	635.1886
670.7810	689.5346	708.1126
783.2736	825.9512	891.5468
941.9189	963.8924	988.9095
1002.5913	1013.2663	1076.3892
1083.7842	1156.7665	1186.6595
1208.4541	1264.9660	1293.5691
1354.5905	1373.6522	1389.2900
1416.1534	1439.9518	1475.7586
1486.8006	1490.9165	1519.2558
1583.1049	1713.1969	2921.0667
2960.8563	3019.9054	3074.2209
3110.1116	3144.0251	3159.2146
3162.5490	3170.0297	3250.6160

ZeroEnergy[kcal/mol] 75.76

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R4-1_ts6-----

Barrier R4-1_ts6 R4-1_ip5 R4-1_ip6

RRHO

Geometry[angstrom] 19

C	-0.0808689739	0.05964287	1.7538745213
C	0.4328348221	-1.3483515959	1.8682553419
C	0.7585842909	-1.9572024817	0.534325069
C	0.6684169441	-1.2697666636	-0.6128790854
C	0.2446903853	0.1293978696	-0.6678692479
C	-0.1786099432	0.7474265072	0.5984789067
C	-0.7221399401	2.1526961689	0.5722558071
C	-0.0867079888	0.7389431137	-1.9966765563
H	-0.3929251664	0.5413950407	2.6763598747
H	-0.2997118473	-1.9758345893	2.4010709759
H	1.3245903719	-1.3711792098	2.5177033378
H	1.0758435512	-2.9951194131	0.5172627132
H	0.9113504239	-1.7552959784	-1.5540073835
H	1.0962289404	0.8232118264	-1.2553504713
H	-1.6455878566	2.2116573541	-0.0143216376
H	-0.0118672879	2.8542107351	0.1190196791
H	-0.9402990514	2.5033429441	1.5821589325
H	-0.5473483527	1.7111418323	-2.0590505729
H	0.0853416784	0.1604826696	-2.8921102044

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1798.6459

WellDepth[kcal/mol] 27.73

WellDepth[kcal/mol] 52.82

End

```

Frequencies[1/cm]  50
84.3489            205.3529
241.7983            296.1474            307.0833
368.8512            390.9442            449.9608
476.1405            525.3327            563.3276
623.8662            697.6091            767.6346
800.4214            802.3039            897.6976
932.7280            967.6852            981.1301
989.2703            1058.8606           1076.0719
1128.8564           1170.3124           1188.2927
1206.8617           1232.0069           1292.8277
1358.8243           1394.2249           1417.8244
1427.5300           1437.8789           1468.4715
1484.3005           1497.3951           1636.2926
1702.2387           2153.6614           2929.7861
2949.9092           3009.7259           3052.5674
3105.2021           3139.5508           3142.8807
3163.7873           3174.3844           3295.7888
ZeroEnergy[kcal/mol] 67.64
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-1_ts7-----
Barrier      R4-1_ts7  R4-1_ip6  R4-1_p9
RRHO
Geometry[angstrom]  19
C  -0.3069206866    -0.0440902403    1.6601790142
C   0.1129968665    -1.3883943615    1.6832351055
C   0.686969351    -1.9365944339    0.522628644
C   0.9336193098    -1.1198232872    -0.5703506336
C   0.5816396282    0.2356283092    -0.5708604752
C  -0.0625785951    0.7770222003    0.5652089758
C  -0.4912922738    2.2242067902    0.5931593814
C   0.8717845461    1.0921347245   -1.7775444375
H  -0.805103365    0.3679699329    2.5314278026
H  -0.220806402   -2.0393704054    2.482098837
H   1.6312463888   -1.2490211226    2.7678547032
H   0.9633951792   -2.9841668021    0.4964575479
H   1.4037118802   -1.5390971406   -1.4542877378
H  -1.185771721    2.4565573898   -0.2208279744
H   0.3644096917    2.8984609387    0.4822470643
H  -0.9863302925    2.4670030901    1.5348248097
H   1.5216166493    1.9371408005   -1.5257706379
H  -0.0445076795    1.5155798422   -2.2030592406
H   1.3662825247    0.5134077752   -2.5594667485
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  749.5964
WellDepth[kcal/mol]  25.81

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WellDepth[kcal/mol]  6.69
End
Frequencies[1/cm]   50
128.2725             162.6343
163.4448             239.2823             301.8517
338.2499             372.7428             417.0147
449.1660             507.3404             550.1829
589.5229             719.9984             742.3354
795.8120             833.7199             877.7505
954.3813             998.9515             1008.4126
1026.8963            1044.2668            1053.2172
1068.9294            1138.7464            1179.1149
1200.3838            1241.5182            1311.7011
1323.3807            1413.3842            1423.9810
1462.1320            1480.1000            1494.1249
1494.8680            1500.7117            1515.6613
1588.2072            1630.8351            3016.2539
3020.2507            3058.4567            3064.7221
3104.0624            3105.6894            3156.1733
3162.2657            3176.4896            3189.4693
ZeroEnergy[kcal/mol] 40.63
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-1_ts8-----
Barrier      R4-1_ts8  R4-1_ip6  R4-1_ip7
RRHO
Geometry[angstrom]  19
C  -0.3331408952    0.0228490573    1.6759758867
C   0.1262410799   -1.4226912864    1.6842998138
C   0.8183853907   -1.8862379974    0.5228008285
C   1.1031861754   -1.048855834    -0.5095487706
C   0.6492601      0.3518905609    -0.5389083165
C  -0.073284765    0.8472987361    0.5134746102
C  -0.6690148014    2.2324069986    0.5698249358
C   1.0060953215    1.1152275219   -1.7862203129
H  -1.0506703233    0.3323027434    2.4242426985
H  -0.2949165204   -2.0989173397    2.4156612139
H   0.7370210452   -0.4613866427    2.2623046808
H   1.1205329572   -2.9276387385    0.4808468165
H   1.6554522656   -1.4189552654   -1.366259675
H  -1.7638495055    2.1768485849    0.5659301372
H  -0.3660803201    2.8677938567   -0.2600290064
H  -0.3806155578    2.7322005348    1.5005139207
H   2.0923771158    1.111798044   -1.9411266367
H   0.6768109419    2.1527840697   -1.7755264039
H   0.5667022953    0.6362823957   -2.6704874208
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart

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ImaginaryFrequency[1/cm]  2459.5415
WellDepth[kcal/mol]  46.37
WellDepth[kcal/mol]  46.37
End
Frequencies[1/cm]  50
51.4307          113.0512
144.7543          185.2882          350.9443
356.9314          374.3007          460.0785
495.5104          533.9059          599.2775
627.4953          705.6579          725.4946
776.6453          819.0901          899.3563
949.0648          967.1857          989.2776
1034.4188         1056.8332         1094.4726
1148.7365         1172.0717         1182.4421
1219.4688         1252.3726         1329.6588
1374.8280         1401.2245         1421.2333
1447.7770         1478.9306         1485.5418
1486.8775         1498.1050         1561.4725
1602.7867         2178.6325         2997.0880
3015.4033         3027.9412         3056.0154
3125.5108         3141.7121         3155.4283
3174.5563         3185.8586         3200.3625
ZeroEnergy[kcal/mol]  61.19
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R4-1_ts16-----
Barrier      R4-1_ts16  R4-1_ip7  R4-1_p9
RRHO
Geometry[angstrom]  19
C  -0.7549505728  -0.2359604923  1.4107613108
C  -0.3944822314  -1.5908515918  1.5434117575
C   0.4033584558  -2.1819184369  0.5793648766
C   0.8062177282  -1.44258324   -0.5347978341
C   0.4045243953  -0.1145923025  -0.7182420136
C  -0.4088661179  0.4931191917  0.2513344562
C  -0.8685553384  1.9204230765  0.1043988407
C   0.8376965036  0.642689938   -1.9503238096
H  -1.4930294127  0.1826251064  2.0860357669
H   0.4418943927  0.5565435211  2.619320213
H  -0.7200646457  -2.150168714  2.4127105578
H   0.7094255373  -3.2171529702  0.6804158207
H   1.4331857687  -1.9102720087  -1.2870232415
H  -1.5274206883  2.2072076111  0.925526695
H  -1.4104481874  2.0775848671  -0.8336747412
H  -0.0203201126  2.6141986966  0.102220458
H   1.4055122944  1.5423826314  -1.6912292757
H  -0.0210619428  0.9704132897  -2.5455923815
H   1.4682341739  0.0226028268  -2.589704456
Core  RigidRotor
SymmetryFactor  1.0

```

```

End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  717.4284
WellDepth[kcal/mol]  25.09
WellDepth[kcal/mol]  5.97
End
Frequencies[1/cm]  50
113.6374          146.3437
167.7003          243.7021          299.6857
302.3970          373.4849          417.7214
500.8936          511.7588          522.3393
587.3996          723.3883          746.0925
768.6729          833.5910          894.1021
967.4676          999.6950          1003.2450
1009.0090         1047.0510          1067.0231
1070.3361         1137.8563          1183.4107
1199.5717         1232.4851          1308.0905
1322.6107         1413.1681          1423.0302
1457.4188         1480.4859          1493.8514
1494.2799         1497.3545          1518.8620
1606.1248         1620.1964          3017.0927
3019.4193         3061.6338          3064.2024
3104.1692         3106.1933          3156.6722
3162.2457         3173.8770          3189.2309
ZeroEnergy[kcal/mol]  39.91
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R4-1_ts9-----
Barrier      R4-1_ts9  R4-1_ip7  R4-1_ip8
RRHO
Geometry[angstrom]  19
C  -0.2684190132  -0.032150337  1.6562463929
C   0.1455778558  -1.4001694345  1.749281932
C   0.9131654921  -1.9713272838  0.7834366075
C   1.2718805199  -1.2174478115  -0.4114119185
C   0.845710342   0.0625184166  -0.6195832294
C   0.0852138327  0.7661922419  0.398704037
C  -0.7153711254  2.0104914099  0.1304519153
C   1.1514382932  0.7713128911  -1.9135202776
H  -1.0145300555  0.3864157161  2.3181968515
H   0.7224007275  0.7804618456  1.5354487365
H  -0.1680061988  -1.9743143708  2.6150578617
H   1.2374662271  -3.0007785742  0.8750388118
H   1.8680493461  -1.706685429  -1.173727391
H  -1.6940894385  1.7709558311  -0.3129899656
H  -0.2029707205  2.6996948957  -0.5434097563
H  -0.916206378  2.5528365152  1.0596388262
H   1.7779323911  0.1518685554  -2.5569945402
H   1.6734712631  1.7181042937  -1.7365187048
H   0.2354706392  1.0117786283  -2.4640321888

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Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 2614.3857
WellDepth[kcal/mol] 45.65
WellDepth[kcal/mol] 44.93
End
Frequencies[1/cm] 50
125.2062          166.6246
187.8251          226.7790          293.1078
320.5804          379.5619          480.7360
493.9315          540.5226          623.1383
654.5944          704.1828          744.5465
805.8434          823.4005          924.1634
952.4316          962.5881        1032.4919
1044.7140         1058.4738          1081.6193
1148.5819         1168.1523          1170.5603
1229.7377         1277.2572          1332.7855
1366.0254         1410.7470          1421.1300
1436.9890         1477.8861          1482.8938
1494.6918         1498.7496          1567.4946
1585.1810         2164.2456          2960.0496
3013.6977         3045.7580          3057.5035
3095.4534         3107.2831          3157.4551
3165.2821         3187.2997          3196.8695
ZeroEnergy[kcal/mol] 60.47
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-1_ts11-----
Barrier      R4-1_ts11  R4-1_ip8  R4-1_p9
RRHO
Geometry[angstrom] 19
C -0.4308805007 -0.1359294974 1.5724458087
C 0.2405256799 -1.3309867302 1.7755545763
C 1.0694253342 -1.8353392625 0.7741475513
C 1.1960783327 -1.145009088 -0.4312077864
C 0.5286060228 0.0550585134 -0.6604517525
C -0.2591444652 0.6168439231 0.3871818184
C -1.1892788527 1.7840610095 0.1161162127
C 0.6808909527 0.7747663602 -1.9743157869
H -1.078632461 0.2591192947 2.3480032976
H 0.1152995371 -1.8724815592 2.7064871498
H 1.600831902 -2.7686837123 0.9216692709
H 1.8230436594 -1.5548250259 -1.2166825598
H 1.0901043476 1.7175159215 1.0193454142
H -2.0550745862 1.4487938859 -0.4666108079
H -0.7020330751 2.5832577319 -0.4434512454
H -1.5600215341 2.2075561073 1.0510307286
H 1.1337440489 1.7627282994 -1.8322658079

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H -0.2840255529 0.9332837104 -2.4665808317
H 1.3170062106 0.2098531181 -2.6577832503
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 763.7764
WellDepth[kcal/mol] 25.33
WellDepth[kcal/mol] 6.93
End
Frequencies[1/cm] 50
157.1210 171.4726
187.5970 253.6161 306.0307
369.0004 421.1700 465.2045
476.6381 535.7205 541.5754
595.3210 715.3169 744.9102
758.9813 833.8656 873.0610
946.7818 987.7281 1000.4932
1009.0231 1046.4275 1066.8619
1071.4868 1144.2751 1183.1960
1202.2758 1229.8575 1310.3176
1319.9728 1412.8370 1420.7374
1463.7162 1479.7775 1490.9113
1494.2979 1505.4540 1513.8714
1594.5523 1631.4296 3014.8394
3021.0014 3060.7933 3088.1463
3103.9207 3118.0602 3155.5456
3161.0503 3173.9252 3187.9217
ZeroEnergy[kcal/mol] 40.87
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-1_ts10-----
Barrier R4-1_ts10 R4-1_ip8 R4-1_p14
RRHO
Geometry[angstrom] 19
C 0.028984712 0.227930249 1.7350698416
C 0.1322959482 -1.15153141 1.758189983
C 0.502872484 -1.8434479666 0.5998567703
C 0.8109895597 -1.1340874983 -0.5670577948
C 0.7176060711 0.2501358637 -0.620120866
C 0.2102989688 0.9446360089 0.5213083475
C -1.8648447696 1.3889001163 -0.0518905781
C 1.0871538907 1.0178781733 -1.8613807316
H -0.2366582866 0.7712900028 2.635244214
H -0.0515196222 -1.6946978097 2.6787635903
H 0.5903720264 -2.9237910289 0.6144117844
H 1.1543225856 -1.6751932824 -1.443590398
H 0.3706662345 2.0162423362 0.5770247191
H -2.2426289721 0.3878837111 -0.2199638003
H -1.7550469479 2.0119993028 -0.9329391981

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H -2.2378085472 1.8919301738 0.8334236057
H 1.7603172203 1.8494821605 -1.6295137113
H 0.2018339892 1.4490898301 -2.3429020979
H 1.5835804551 0.3772520673 -2.5930036797
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 500.9671
WellDepth[kcal/mol] 21.51
WellDepth[kcal/mol] 11.95
End
Frequencies[1/cm] 50
79.3892 108.8114
123.4804 169.2504 212.7701
344.7478 399.0013 483.9654
519.1218 560.9729 582.2655
632.8656 689.9117 736.9861
788.1312 848.3555 873.2666
932.7609 972.7763 980.3007
1000.9158 1020.5266 1042.9941
1057.0384 1091.1885 1175.8363
1187.4569 1211.4681 1321.7443
1344.0370 1412.4670 1426.0821
1427.6026 1447.8747 1484.5346
1498.3273 1518.1480 1575.1047
1609.4624 3013.0814 3058.5110
3076.8599 3099.6570 3146.6222
3152.3513 3161.6453 3175.2949
3186.7609 3223.3032 3237.3628
ZeroEnergy[kcal/mol] 37.05
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-1_ts12-----
Barrier R4-1_ts12 R4-1_ip2 R4-1_ip10
RRHO
Geometry[angstrom] 19
C -1.5275584461 0.1552040289 1.2338579414
C -0.8480705705 -1.1752457246 1.3029924053
C 0.015540458 -1.4959006969 0.1069574301
C 0.5466750103 -0.6105774537 -0.746941482
C 0.4325032402 0.8560302844 -0.6637207773
C 0.2743408458 1.4966164592 0.674096376
C 1.1690254417 1.3094175975 1.6846812216
C 0.4965364267 1.6106799584 -1.7713750822
H -1.8491642248 0.6199551196 2.1587851133
H -2.1354446134 0.370064081 0.3607938184
H -1.5972070931 -1.977595223 1.4018094836
H -0.2438511425 -1.2390014116 2.2189677899
H 0.1907130189 -2.5518815049 -0.0814443107

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H 1.0927207862 -0.9917599838 -1.6059100449
H -0.3495901133 2.3850583762 0.6997749823
H 1.9080837326 0.5176190935 1.647949384
H 1.1316826868 1.9155771387 2.5819920924
H 0.4043837077 2.6900754839 -1.7300199204
H 0.6441678488 1.1649853773 -2.7490824208
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 396.1909
WellDepth[kcal/mol] 29.87
WellDepth[kcal/mol] 8.36
End
Frequencies[1/cm] 50
87.0162 157.3860
223.0050 230.6226 341.1264
360.0530 431.9594 450.5133
529.5498 570.5596 594.2878
706.8481 729.7318 757.8966
791.9278 795.4323 839.4172
877.1211 903.4891 910.8045
961.4814 979.8443 998.3212
1051.3536 1066.3889 1101.0767
1216.5110 1245.6355 1281.1338
1323.3712 1357.3153 1385.8344
1420.8808 1449.1810 1458.4542
1466.7628 1549.1750 1652.7741
1695.2849 2951.7050 2995.0945
3119.0211 3129.6522 3132.8467
3136.2879 3145.4844 3153.2434
3216.1030 3216.2100 3226.9313
ZeroEnergy[kcal/mol] 68.59
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-1_ts13-----
Barrier R4-1_ts13 R4-1_ip10 R4-1_p11
RRHO
Geometry[angstrom] 19
C -1.1089734187 -0.1366640918 2.3967503009
C -0.7670260463 -1.0901079121 1.5041220307
C -0.8176461463 -0.191295651 -0.6962058486
C 0.2467253956 -0.0407624569 -1.4588620117
C 1.669424537 -0.1139124133 -1.0407094198
C 2.6069829384 -0.8744982368 -1.8784390883
C 2.2839188328 -1.6462341144 -2.9202611314
C 2.1105439026 0.5306727623 0.0531239393
H -0.3666551996 0.5216714768 2.8342759243
H -2.1423869165 0.0430321383 2.6717422827
H -1.4991062304 -1.8063381021 1.149647905

```

```

H  0.2711058951   -1.328806645    1.3106267984
H -1.8702168104   -0.1159945341   -0.9359715129
H  0.0895287722    0.156784798   -2.5255316206
H  3.6532296499   -0.787577914   -1.5943168103
H  1.2569947216   -1.787167122   -3.2377551139
H  3.0451800294   -2.1730001465   -3.4832024587
H  3.1527837572    0.480087258    0.3498502622
H  1.4441583364    1.1276609065    0.6620605727
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 287.6732
WellDepth[kcal/mol] 36.81
WellDepth[kcal/mol] 3.83
End
Frequencies[1/cm] 50
38.7543          39.7876
116.6729         117.5007         157.2033
232.8755         269.5008         302.2537
362.7282         403.1147         512.4639
539.6230         644.9418         755.4994
771.5267         792.8581         826.9911
886.7419         895.5045         913.1345
931.0253         939.6728         945.8119
1011.6635        1026.8544        1027.9130
1059.4837        1236.6461        1240.2097
1313.1382        1325.1607        1328.6865
1420.5625        1459.4739        1466.6572
1591.7216        1642.7187        1652.1867
1689.1859        3021.4149        3129.9669
3132.0664        3139.5867        3141.6089
3144.1853        3204.2666        3206.2153
3224.0344        3233.2219        3234.7114
ZeroEnergy[kcal/mol] 97.04
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```

R4_seconadary_c8h11_4

```
!-----c10h15_R4-3_rp1-----
Well          R4-3_rp1
Species
RRHO
Geometry[angstrom]  19
C  -1.3041919299   -1.1811229235    1.0454971757
C  -0.0993392872   -0.9173711578    0.2017605849
C  -0.311163397    0.5137639149   -0.2492333448
C  -1.4772585662    1.0070032493    0.1652890297
C  -2.2688468496   -0.0281162048    0.9456488142
C  1.3390459637    -0.833249579    0.7764426893
C  0.9765806494    1.0873862254   -0.7773515486
C  2.0609743524    0.0933962149   -0.2381605862
H  -1.5517986602   -2.1369149183    1.4902938408
H  -0.062351725   -1.603955217   -0.6650007611
H  -1.8153797412    2.029703791    0.0409882724
H  -2.5795669404    0.3575518752    1.9293879556
H  -3.2095031922   -0.3132142022    0.4430335926
H  1.8292869915   -1.804329071    0.8794119593
H  1.3025735979   -0.3663831846    1.7655461492
H  1.1357591711    2.1078339685   -0.4196202577
H  0.995727081     1.1277263312   -1.8712707886
H  2.455452653    -0.5050566474   -1.0644918086
H  2.9101738289    0.6120785352    0.2116120319
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
94.5728           180.1562           233.7398
328.3175           363.0075           418.4472
558.1997           609.8309           661.1569
733.0000           788.3316           814.8693
832.8870           885.5632           897.3057
925.9003           935.1134           956.4175
982.7315           1003.1691          1041.1462
1061.2483           1127.2853          1130.1328
1156.5365           1181.0231          1226.9334
1258.9582           1270.5069          1285.7166
1293.9730           1310.6925          1334.1426
1335.3936           1360.5091          1463.8022
1480.7496           1493.1603          1507.9252
1719.7058           2896.9889          2929.3938
2960.2053           3027.1120          3035.0643
3042.4400           3063.3227          3080.5449
3092.6024           3175.9033          3190.1978
ZeroEnergy[kcal/mol]  34.42
ElectronicLevels[1/cm]  1
0  2
End
```

```

End
!-----
!-----c10h15_R4-3_ts2-----
Barrier      R4-3_ts2  R4-3_rp1  R4-3_ip2
RRHO
Geometry[angstrom]  19
C  -1.3032585011  -1.1935367298  0.8534076455
C  -0.2070343294  -1.0498839318  0.0153402727
C  -0.1430393036  0.3733535779  -0.3995173782
C  -1.1305353118  1.0628354706  0.1919349504
C  -1.9653280643  0.143952923  1.0531376807
C  1.8508582987  -0.8664946143  0.7339463319
C  1.1419985717  0.8235987717  -1.011025642
C  2.2087792814  0.4468427741  0.0668235592
H  -1.6964585863  -2.1251416813  1.2375922891
H  0.155682374  -1.8616993927  -0.6042847345
H  -1.2616788536  2.1375445391  0.1620581997
H  -1.9649034396  0.4802090308  2.1014645294
H  -3.0234572011  0.1096666757  0.7554205285
H  2.2741787271  -1.7753098652  0.3165960003
H  1.7548363243  -0.8825490966  1.8136054498
H  1.1609940457  1.8916922423  -1.2377910527
H  1.3441085749  0.279887228  -1.9412233819
H  3.2069227123  0.4060118578  -0.3844878387
H  2.2251086809  1.2445422207  0.8141375909
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  550.9954
WellDepth[kcal/mol]  24.14
WellDepth[kcal/mol]  15.54
End
Frequencies[1/cm]  50
101.1695          152.9462
278.4943          347.9792          365.5795
482.5798          565.4860          636.3548
645.5782          674.4605          765.7986
774.2323          822.2011          833.9535
875.9447          903.7048          913.2984
920.8085          938.9893          952.6821
981.7788          1033.7459          1083.6658
1094.0531         1124.8271          1165.6892
1193.9509         1225.4454          1272.1339
1288.2497         1324.4520          1339.3906
1380.5935         1414.2449          1444.9557
1464.5537         1486.4154          1500.2023
1679.6060         2978.1926          2996.7646
3012.3460         3020.1344          3063.8412
3087.0617         3113.6465          3159.4543
3190.6264         3204.5386          3206.9474
ZeroEnergy[kcal/mol]  58.56

```

```

ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R4-3_ip2-----
Well          R4-3_ip2
Species
RRHO
Geometry[angstrom] 19
C  -1.7152899546  -1.2421934639  0.6152716783
C  -0.5515093793  -1.1567235285  -0.0528383264
C  -0.1928740643  0.2612667867  -0.254926622
C  -1.1596123309  1.023377494  0.2985936704
C  -2.2178041751  0.1455870379  0.9068311658
C  2.7658643677  -0.8577676196  0.1052812743
C  1.047938039  0.7390634879  -0.9514096211
C  2.3593707123  0.5561616806  -0.1220617019
H  -2.2326182912  -2.1470554142  0.9044128568
H  0.0481326052  -1.9872234715  -0.4032581847
H  -1.1918363211  2.1052745539  0.3113414701
H  -2.331769463  0.3220149463  1.9853468745
H  -3.2083652551  0.3228188406  0.4657773606
H  3.1622050798  -1.4516993177  -0.7109848341
H  2.6035885367  -1.3521729517  1.0542786497
H  0.9408474376  1.8026801406  -1.1859275536
H  1.1652890199  0.2136196168  -1.9066670781
H  3.1530217367  1.0833800634  -0.6689265959
H  2.2317646996  1.0741601185  0.8331075172
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 51
46.3955 105.0382 114.3542
144.9681 275.3769 311.2770
367.6062 411.8610 531.4571
582.1672 650.5713 710.8031
758.5528 814.7833 822.8457
856.0310 911.7991 925.9281
928.9372 943.1418 953.1014
991.4536 1065.6533 1092.5560
1102.9196 1125.0767 1177.3649
1217.4305 1253.8471 1268.5268
1300.2433 1338.0098 1360.2825
1395.1246 1419.6832 1463.3194
1483.4954 1489.1340 1572.6311
1666.2060 2987.3328 3007.1679
3014.0382 3027.5138 3053.2910
3065.0975 3132.8450 3191.3786
3198.5603 3216.0164 3236.6360
ZeroEnergy[kcal/mol] 43.02
ElectronicLevels[1/cm] 1
0 2

```

```

End
End
!-----
!-----c10h15_R4-3_ts3-----
Barrier      R4-3_ts3  R4-3_ip2  R4-1_p13
RRHO
Geometry[angstrom]  19
C  -1.698437986  -1.2423520564  0.5700513154
C  -0.5748516696  -1.1889683567  -0.1628723935
C  -0.131573537  0.2135119873  -0.3102109613
C  -1.0234994309  1.0028793851  0.3667788556
C  -2.0983540102  0.1514758699  0.9784776943
C  3.0914824392  -0.84735432  0.5665490126
C  1.0575857738  0.6209543774  -0.9978058292
C  2.7261025424  0.4582719798  0.3412676673
H  -2.2531540998  -2.131382241  0.8390348065
H  -0.0505481025  -2.0318830139  -0.5957869333
H  -0.9842312845  2.0812026043  0.4475048699
H  -2.1461627487  0.2593452605  2.071696385
H  -3.0998633259  0.415159269  0.6094100772
H  3.7841060808  -1.3610663125  -0.0907539724
H  2.6237739403  -1.4384774834  1.3452213106
H  1.1767169951  1.680798954  -1.1997650756
H  1.4474950958  -0.0309458034  -1.7704636725
H  3.3434930273  1.0693173879  -0.3097546611
H  2.1955223005  1.002422512  1.1144125045
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  592.923
WellDepth[kcal/mol]  22.47
WellDepth[kcal/mol]  14.1
End
Frequencies[1/cm]  50
52.2143          76.0945
103.4484         235.6441         287.7307
348.1051         380.9514         405.6017
610.1117         644.0202         689.6370
741.0624         749.2892         793.0007
812.5499         813.3752         847.7118
918.6683         921.9433         940.4628
955.1312         976.3012        1010.9110
1026.1606        1039.1612        1105.4771
1123.2126        1229.7770        1243.8973
1262.4174        1267.5510        1304.2109
1391.2630        1423.8057        1463.2851
1481.0201        1514.4530        1554.4784
1623.8823        2996.1872        3012.3149
3113.6965        3122.0723        3132.7104
3188.0017        3192.8248        3202.8401
3208.7015        3213.7021        3225.2773

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```

ZeroEnergy[kcal/mol] 65.49
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c2h4_c6h7_R4-1_p13-----
Bimolecular R4-1_p13
Fragment c6h7
RRHO
Geometry[angstrom] 13
C -0.5194108697 -1.2037450174 0.676593069
C 0.5261795571 -1.0702094516 -0.150519562
C 0.7454530747 0.3568200979 -0.4793111934
C -0.2405683459 1.0822594629 0.2065586089
C -1.1141916122 0.1481423723 0.9897637854
C 1.7378005645 0.8491720647 -1.3056311662
H -0.9037441313 -2.1321677625 1.0784514411
H 1.1410530257 -1.8728673995 -0.5386966542
H -0.3603241565 2.1569557376 0.1810204193
H -1.0988913384 0.3648489283 2.0682495049
H -2.1710472315 0.2124544278 0.6913662525
H 1.8313003338 1.9111318135 -1.4968543159
H 2.4492471296 0.1890647261 -1.7860431895
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 33
217.4060 351.0584 356.4188
531.7375 585.7556 643.3277
655.2255 743.3614 773.2253
791.6226 915.1778 918.3381
939.2190 953.0315 960.4209
1015.6686 1107.5646 1125.5911
1250.6221 1273.3288 1319.5816
1365.4020 1429.5279 1442.8506
1513.6175 1629.5271 2985.3119
2996.8492 3143.4675 3187.1535
3207.0999 3211.9826 3235.0183
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment c2h4
RRHO
Geometry[angstrom] 6
C 0.0 0.6634900906 0.0
C 0.0 -0.6634900906 0.0
H 0.0 1.23462754 -0.9225248038
H 0.0 1.23462754 0.9225248038
H 0.0 -1.23462754 0.9225248038
H 0.0 -1.23462754 -0.9225248038
Core RigidRotor

```

```

SymmetryFactor 4
End
Frequencies[1/cm] 12
834.2929          972.9227          974.1218
1066.8559         1238.5875         1379.4650
1472.0483         1691.5384         3121.2072
3136.3255         3192.3844         3220.8390
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 51.39
End
End

```

R4_seconadary_c6h7

```
!-----R4-1_rp11-----
Well          rp11
Species
RRHO
Geometry[angstrom]  13
C  -1.6342206836   0.3745969637   1.0301065855
C  -0.6684592972   0.4795520041   0.1490075986
C   0.7864649132   0.4243344877   0.4425933957
C   1.674212993   -0.2288658664   -0.5280224116
C   1.2979137387   -0.919787224   -1.6080859988
C   1.2912713298   0.9763528068   1.5590407324
H  -2.7138001123   0.3912803474   1.0350048309
H  -0.936983324   0.6212102457   -0.9038606085
H   2.7359575404   -0.1311446455   -0.3139880794
H   0.2561725338   -1.074573182   -1.8648812003
H   2.0316921394   -1.3677321321   -2.2673769997
H   2.352682154   0.9279702451   1.7755440519
H   0.6566590749   1.4862779495   2.2725791032
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  33
102.3394          147.4103          246.2025
307.1517          397.4239          499.3510
529.5578          630.1924          721.8462
736.7550          779.8269          862.9489
893.4548          930.0291          937.1562
979.5734          1026.2951         1058.9940
1236.5748         1325.8423          1326.6601
1420.3003         1461.0189          1639.6876
1658.5517         1690.7905          3026.1566
3133.8388         3142.1244          3145.2063
3224.1420         3232.9226          3240.9830
ZeroEnergy[kcal/mol]  54.53
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----R4-1_ip13-----
Well          W6
Species
RRHO
Geometry[angstrom]  13
C  -0.5194108697   -1.2037450174   0.676593069
C   0.5261795571   -1.0702094516   -0.150519562
C   0.7454530747   0.3568200979   -0.4793111934
C  -0.2405683459   1.0822594629   0.2065586089
C  -1.1141916122   0.1481423723   0.9897637854
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C 1.7378005645 0.8491720647 -1.3056311662
H -0.9037441313 -2.1321677625 1.0784514411
H 1.1410530257 -1.8728673995 -0.5386966542
H -0.3603241565 2.1569557376 0.1810204193
H -1.0988913384 0.3648489283 2.0682495049
H -2.1710472315 0.2124544278 0.6913662525
H 1.8313003338 1.9111318135 -1.4968543159
H 2.4492471296 0.1890647261 -1.7860431895
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 33
217.4060 351.0584 356.4188
531.7375 585.7556 643.3277
655.2255 743.3614 773.2253
791.6226 915.1778 918.3381
939.2190 953.0315 960.4209
1015.6686 1107.5646 1125.5911
1250.6221 1273.3288 1319.5816
1365.4020 1429.5279 1442.8506
1513.6175 1629.5271 2985.3119
2996.8492 3143.4675 3187.1535
3207.0999 3211.9826 3235.0183
ZeroEnergy[kcal/mol] 12.7
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
Well W1 # c5h5ch2
Species
RRHO
Geometry[angstrom] 13
C -1.364972 0.748558 -0.168119
C -1.384099 -0.720402 -0.16218
C -0.169116 -1.180172 0.184756
C 0.767117 -0.014015 0.439266
C -0.139050 1.179473 0.177520
C 1.991174 -0.024386 -0.422538
H -2.216661 1.371894 -0.410131
H -2.252074 -1.322899 -0.398707
H 0.140320 -2.212656 0.270572
H 1.064296 -0.012078 1.497938
H 0.198733 2.203497 0.256214
H 2.976650 0.151805 -0.012012
H 1.882414 -0.113898 -1.496100
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 33
60.9976 160.1015 293.1123
491.5671 547.3324 566.1844

```

721.1503	727.4514	778.3224
811.5290	864.9942	953.3920
956.5102	990.9784	1004.7536
1020.2443	1091.5782	1110.1930
1139.7085	1206.2049	1278.9374
1302.5104	1390.8785	1451.1448
1547.2416	1635.2485	3001.3014
3141.0117	3185.4404	3196.6833
3218.5870	3223.9912	3250.9220

ZeroEnergy[kcal/mol] 28.3

ElectronicLevels[1/cm] 1

0 2

End

End

Well W2 # c5h5ch2re

Species

RRHO

Geometry[angstrom] 13

C	-1.364144	0.757752	-0.172195
C	-1.393542	-0.714224	-0.162711
C	-0.171147	-1.182705	0.192984
C	0.769714	-0.021058	0.446435
C	-0.124788	1.181924	0.180230
C	1.986718	-0.037418	-0.429980
H	-2.212107	1.394130	-0.422195
H	-2.266616	-1.318819	-0.404483
H	0.130960	-2.224157	0.281796
H	1.076497	-0.016780	1.507281
H	0.221555	2.210428	0.256189
H	2.965341	0.242065	-0.046151
H	1.867505	-0.192489	-1.501021

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 33

86.2208	153.8544	293.2473
496.5792	544.6054	562.5519
708.0313	715.3995	770.4084
807.5088	871.1570	917.5117
931.2717	986.3069	1011.2697
1023.2097	1092.4194	1098.8227
1143.0551	1197.6653	1273.1984
1295.6178	1389.0190	1456.9709
1546.5693	1617.4108	3037.2028
3171.6441	3218.2848	3228.6474
3247.7819	3253.7793	3292.1012

ZeroEnergy[kcal/mol] 30.2

ElectronicLevels[1/cm] 1

0 2

End

End

Well W3 # c6h6h

```

Species
RRHO
  Geometry[angstrom] 13
C      -0.741434      1.229167      -0.000070
C      -1.460677      -0.000001      -0.000068
C      -0.741432      -1.229168      0.000000
C      0.626077      -1.255838      0.000064
C      1.450993      0.000001      0.000070
C      0.626075      1.255839      -0.000007
H      -1.296109      2.169181      -0.000124
H      -2.549546      -0.000002      -0.000119
H      -1.296106      -2.169182      -0.000001
H      1.153743      -2.211162      0.000115
H      2.138378      -0.000023      -0.870363
H      2.138289      0.000026      0.870574
H      1.153740      2.211163      -0.000011
  Core RigidRotor
  SymmetryFactor      1
End
  Frequencies[1/cm] 33
159.6783      387.1462      517.6056
561.0687      587.3326      630.9200
730.5513      767.0194      882.9686
930.2648      968.4006      972.5955
975.3739      985.8838      992.4918
1099.5925      1161.4210      1173.8340
1199.1125      1314.7290      1354.7573
1411.4923      1427.8888      1448.5068
1555.0415      1637.2268      2951.2171
2953.0510      3184.6036      3186.4225
3203.7024      3205.4443      3227.7114
  ZeroEnergy[kcal/mol] 3.0
  ElectronicLevels[1/cm] 1
    0    2
End
End
Well      W4 # c5h4ch3
Species
RRHO
  Geometry[angstrom] 13
C      -1.489683      0.737796      0.000188
C      -1.499521      -0.736573      0.000179
C      -0.197096      -1.166129      0.000115
C      0.665464      0.017404      -0.000673
C      -0.169657      1.171024      -0.000470
C      2.155436      -0.010247      0.000176
H      -2.377624      1.367523      0.000382
H      -2.393687      -1.355951      0.000402
H      0.155604      -2.194998      0.000213
H      0.178322      2.200751      -0.000884
H      2.578624      1.001132      -0.010111
H      2.535187      -0.558757      -0.876449

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```

H                2.533913   -0.539355   0.889363
      Core  RigidRotor
      SymmetryFactor      1
    End
    Frequencies[1/cm]      33
      90.0813      216.2360      325.6366
     517.1729      575.0118      593.5363
     643.8622      691.0305      717.7722
     853.5954      870.2544      913.2601
     953.3981     1010.1798     1016.3823
    1043.8392     1085.9015     1173.3159
    1268.8397     1305.5415     1389.7391
    1423.5112     1460.6766     1463.2034
    1483.3719     1564.7529     3031.2092
    3085.6452     3144.7260     3230.1353
    3237.6115     3252.7389     3260.4127
      ZeroEnergy[kcal/mol]      0.
      ElectronicLevels[1/cm]      1
        0      2
    End
  End
Well      W5  # c5h5ch2-1
  Species
    RRHO
      Geometry[angstrom]      13
      C      -1.432709      0.758689      -0.000001
      C      -0.071166      1.181406      0.000003
      C      0.785055      0.036842      0.000002
      C      -0.115366     -1.194587      0.000005
      C      -1.506877     -0.614485     -0.000006
      C      2.151732      0.025950     -0.000004
      H      -2.289299      1.431972     -0.000004
      H      0.273725      2.213844      0.000008
      H      0.069127     -1.825138     -0.884194
      H      0.069113     -1.825114      0.884224
      H      -2.419081     -1.207710     -0.000011
      H      2.713871     -0.907276     -0.000007
      H      2.718535      0.956537     -0.000006
      Core  RigidRotor
      SymmetryFactor      1
    End
    Frequencies[1/cm] 33
      178.3417      352.7408      393.4581
      528.0027      620.8534      636.2520
      661.4179      769.9704      816.4639
      840.4704      860.0362      919.3815
      940.4895      947.3396      983.1769
     1030.3228     1110.2253     1137.5931
     1246.9864     1268.7020     1304.3498
     1393.9535     1417.5446     1434.4435
     1521.6063     1580.8751     3045.7111
     3081.5851     3166.2739     3219.0758

```

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3235.5746          3248.7325          3265.3633
      ZeroEnergy[kcal/mol]      7.4
      ElectronicLevels[1/cm]      1
      0      2
End
End
!-----c2h2_c4h5_R4-1_p12-----
Bimolecular      R4-1_p12
Fragment          c4h5
RRHO
Geometry[angstrom]      9
C  -0.5345759419      0.4716807441      0.4437914556
C  0.2022891521      -0.0780162834      -0.5433540005
C  -0.2499806701      -1.0131859709      -1.4714176235
C  -1.2432774256      0.99928407      1.395613925
H  1.2401300465      0.246848575      -0.6096525431
H  -1.2710502359      -1.3717114719      -1.4538092776
H  0.4157134721      -1.4001091644      -2.2310578295
H  -1.3069647183      0.5471184031      2.3849964361
H  -1.8087406788      1.9193940983      1.2507904574
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]      21
205.8906          213.4010          495.6577
524.8872          573.1273          741.9547
883.8388          907.3733          937.4436
980.9351          1090.1841          1194.4025
1377.0619          1449.1618          1492.6556
1909.4944          3068.2632          3111.3313
3126.6213          3152.0506          3252.3914
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]      1
0      2
End
Fragment          c2h2
RRHO
Geometry[angstrom]      4
C  0.0      0.0      0.5990703976
C  0.0      0.0      -0.5990703976
H  0.0      0.0      1.6619081422
H  0.0      0.0      -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]      7
642.0679          642.0679          772.6955
772.6955          2069.5209          3420.9272
3523.7963
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]      1
0      1

```

```

End
GroundEnergy[kcal/mol] 79.86
End
!-----
Bimolecular      P1      # C5H4CH2 + H
      Fragment      C5H4CH2
      RRHO
      Geometry[angstrom]      12
C              -1.411784      -0.738890      -0.000002
C              -1.411785      0.738889      -0.000003
C              -0.122752      1.182636      0.000005
C              0.759598      0.000000      0.000000
C              -0.122750      -1.182636      0.000004
C              2.111739      0.000001      -0.000002
H              -2.307349      -1.357984      -0.000005
H              -2.307351      1.357981      -0.000006
H              0.223509      2.213544      0.000007
H              0.223513      -2.213542      0.000007
H              2.677039      -0.932467      -0.000007
H              2.677040      0.932468      -0.000006
      Core      RigidRotor
      SymmetryFactor      2
      End
      Frequencies[1/cm]      30
209.9252      342.4908      487.3855
633.2846      676.7650      683.7378
771.1438      782.7335      806.3938
910.6074      910.8208      911.0513
962.3473      969.4692      1010.8213
1089.7621      1092.6942      1246.8407
1338.5000      1359.9118      1450.0208
1520.7911      1593.1266      1696.3680
3163.4486      3224.4497      3233.9633
3251.1676      3256.9718      3261.8820
      ZeroEnergy[kcal/mol]      0.
      ElectronicLevels[1/cm]      1
      0      1
      End
      Fragment      H
      Atom
      Mass[amu]      1
      ElectronicLevels[1/cm]      1
      0      2
      End
      GroundEnergy[kcal/mol]      54.8
End
Bimolecular      P2      # C6H6 + H
      Fragment      C6H6
      RRHO
      Geometry[angstrom]      12
C              1.008657      0.973075      -0.000001
C              1.347069      -0.386963      0.000000

```

```

C          0.338413   -1.360050   0.000001
C          -1.008657  -0.973075  -0.000001
C          -1.347068   0.386963   0.000001
C          -0.338413   1.360050   0.000000
H          1.793539   1.730361  -0.000008
H          2.395325  -0.688041   0.000005
H          0.601729  -2.418428   0.000002
H          -1.793539  -1.730361  -0.000008
H          -2.395324   0.688041   0.000002
H          -0.601730   2.418428   0.000005

      Core   RigidRotor
      SymmetryFactor      12
      End
      Frequencies[1/cm]      30
408.1607          408.5826          611.9580
612.1494          684.0933          696.2322
856.5484          856.9511          970.7189
970.8519          980.0820        1000.2940
1012.2348         1057.2112        1057.5452
1165.2677         1190.3052        1190.4149
1352.2873         1376.6220        1491.9339
1492.2837         1635.0663        1635.2633
3188.3929         3197.3357        3197.4396
3212.7743         3212.8770        3222.4207

      ZeroEnergy[kcal/mol]      0.
      ElectronicLevels[1/cm]    1
      0      1
      End
      Fragment      H
      Atom
      Mass[amu]    1
      ElectronicLevels[1/cm]    1
      0      2
      End
      GroundEnergy[kcal/mol]      23.4
End
!-----R4-1_ts14-----
Barrier      ts14   rp11   R4-1_p12
RRHO
Geometry[angstrom]    13
C  -1.5412463206   0.2218921312   0.6294949837
C  -0.7169315647   0.7667581602  -0.0805185119
C   1.4657660343   0.403099878   0.5879106242
C   2.2328823464  -0.3465411543  -0.368724917
C   1.7361985847  -1.1250243848  -1.3375266836
C   1.7522552536   1.0179322334   1.7196334186
H  -2.1002572241  -0.3257707214   1.3498548429
H  -0.3468643257   1.3657380659  -0.8812906751
H   3.3188738556  -0.250066405  -0.2761179942
H   0.6678696511  -1.2503916488  -1.4683651598
H   2.3904651234  -1.6623723815  -2.0133526728
H   2.7628866701   0.9986061829   2.1351591897

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```

H 1.003384916 1.5567420441 2.2906975556
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 398.5695
WellDepth[kcal/mol] 38.96
WellDepth[kcal/mol] 13.63
End
Frequencies[1/cm] 32
24.8647 74.0051
136.7390 164.4146 246.9546
296.5341 435.6274 503.2837
555.9584 649.4623 728.3598
765.1726 770.7877 877.8429
896.0878 948.2202 992.3449
999.7191 1142.7886 1304.6606
1402.4590 1445.9011 1647.1971
1704.2362 1926.0198 3050.3143
3055.7339 3144.5445 3171.8568
3232.7222 3385.0033 3475.6122
ZeroEnergy[kcal/mol] 93.49
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R4-1_ts15-----
Barrier ts15 rp11 W6
RRHO
Geometry[angstrom] 13
C -1.4210342509 0.0793930809 -0.8604177801
C -0.9525163602 0.3826428642 0.3378475812
C 0.5103716583 0.3843700669 0.552925225
C 1.2085271724 -0.0155465651 -0.6673464261
C 0.5686640285 -0.8167806024 -1.5739390567
C 1.0988560165 0.797107097 1.6919428129
H -2.4117799862 -0.0635568255 -1.2703058894
H -1.6029005313 0.6605442653 1.1683018035
H 2.1200193409 0.5065739502 -0.9404583243
H -0.0777903449 -1.6279734905 -1.2626226374
H 0.9282717302 -0.8852081758 -2.5964878113
H 2.1767207775 0.8013054233 1.8024315666
H 0.5127577492 1.1399449117 2.5368229361
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 584.6471
WellDepth[kcal/mol] 11.47
WellDepth[kcal/mol] 53.3
End
Frequencies[1/cm] 32

```

177.5257	309.0104	
358.9577	429.0470	530.0012
608.4019	651.0868	725.5552
734.1957	779.0326	849.4751
871.1697	882.1419	903.2647
942.3433	969.3004	1048.0900
1210.9043	1255.8748	1309.0157
1399.0072	1448.7109	1550.9495
1607.6854	1645.5267	3091.8680
3125.4452	3139.3430	3159.8571
3201.5431	3218.3082	3224.8107

ZeroEnergy[kcal/mol] 66.0

ElectronicLevels[1/cm] 1

0 2

End

!-----

Barrier B1 P1 W1 # ts1

RRHO

Geometry[angstrom] 13 #

C	-1.422817	0.735789	-0.077127
C	-1.422812	-0.735799	-0.077115
C	-0.141033	-1.185399	0.024968
C	0.752868	-0.000003	0.068811
C	-0.141042	1.185396	0.024949
C	2.093390	-0.000005	-0.169375
H	-2.315390	1.354771	-0.146509
H	-2.315381	-1.354787	-0.146489
H	0.205056	-2.215675	0.044289
H	0.607970	0.000155	1.936167
H	0.205045	2.215673	0.044252
H	2.650688	0.932662	-0.251193
H	2.650686	-0.932675	-0.251179

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1003.7215

WellDepth[kcal/mol] 5

WellDepth[kcal/mol] 21.5

End

Frequencies[1/cm] 32

240.2869	243.5512	
346.2059	452.7516	496.7080
597.0245	665.8483	691.4094
741.0524	765.9813	819.0018
903.9866	911.5057	912.2411
936.8190	961.1865	1017.9291
1091.3631	1098.0042	1248.3914
1351.0315	1360.1444	1447.0110
1518.4367	1639.6222	1657.0783
3169.4892	3228.1585	3238.5350
3257.3254	3262.2711	3272.3080

```

ZeroEnergy[kcal/mol]          59.8
ElectronicLevels[1/cm]       1
  0    2
End
Barrier      B2    W2    W1    #    ts2
RRHO
  Geometry[angstrom]          13
C              0.977226      1.041067      0.090817
C              1.462552      -0.318236      0.221839
C              0.492035      -1.198916     -0.160902
C             -0.741122      -0.436712     -0.536761
C             -0.320721      0.999790     -0.407684
C             -1.615273     -0.120002      0.651375
H              1.522974      1.937985      0.374844
H              2.446106     -0.589377      0.603250
H              0.553471     -2.284555     -0.143660
H             -1.286070     -0.751012     -1.432735
H             -0.933490      1.840880     -0.717566
H             -2.616938      0.279690      0.509539
H             -1.214237     -0.235560      1.654225
Core      RigidRotor
  SymmetryFactor      0.5
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]    583.3573
  WellDepth[kcal/mol]        8.3
  WellDepth[kcal/mol]        6.4
End
Frequencies[1/cm]          32
285.8985              425.5000
526.4511              576.5394      621.4208
722.2603              728.9065      787.5781
819.3949              840.5185      889.9330
937.4444              953.8269     1017.3173
1038.7812             1073.4360      1101.2489
1112.0776             1181.8657      1275.1306
1315.0544             1386.8979      1411.9658
1441.6394             1580.3423      3130.7315
3178.5507             3223.7165      3241.5568
3253.1758             3267.9946      3309.9545
ZeroEnergy[kcal/mol]          36.6
ElectronicLevels[1/cm]       1
  0    2
End
Barrier      B3    W3    W2    #    ts3
RRHO
  Geometry[angstrom]          13
C              0.651681      1.209438     -0.069116
C              1.460341      0.043729      0.227600
C              0.812268     -1.126821     -0.064627
C             -0.611921     -0.975033     -0.391337
C             -0.719124      0.990900     -0.227199

```

C	-1.405650	-0.142641	0.526790
H	1.106708	2.160261	-0.349372
H	2.501480	0.102058	0.540664
H	1.293535	-2.105475	-0.069891
H	-1.066531	-1.444979	-1.264425
H	-1.340488	1.659127	-0.823612
H	-2.485879	-0.158750	0.366014
H	-1.134392	-0.209673	1.587955
Core RigidRotor			
SymmetryFactor 1			
End			
Tunneling Eckart			
ImaginaryFrequency[1/cm] 800.5544			
WellDepth[kcal/mol] 36.7			
WellDepth[kcal/mol] 9.5			
End			
Frequencies[1/cm] 32			
345.3661	393.3140		
523.4498	596.6085	666.2770	
697.8606	727.7895	801.7810	
828.9799	888.8627	910.2278	
968.7541	1025.1631	1059.3179	
1087.1913	1104.2097	1164.4481	
1178.8770	1190.0066	1307.5833	
1389.2622	1403.6745	1440.3814	
1476.5829	1575.0335	3077.6741	
3180.6714	3194.9702	3199.2616	
3208.7528	3212.1304	3234.7644	
ZeroEnergy[kcal/mol] 39.7			
ElectronicLevels[1/cm] 1			
0 2			
End			
Barrier	B4	P2	W3 # ts4
RRHO			
Geometry[angstrom] 13			
C	0.742072	-1.214542	-0.003862
C	1.440978	0.000000	0.057598
C	0.742073	1.214541	-0.003863
C	-0.647118	1.220600	-0.094007
C	-1.366135	0.000000	-0.058346
C	-0.647119	-1.220600	-0.094007
H	1.289937	-2.157328	0.004361
H	2.528757	-0.000001	0.128772
H	1.289939	2.157328	0.004361
H	-1.190540	2.164040	-0.146704
H	-2.431760	0.000001	-0.287115
H	-1.884295	0.000001	1.621950
H	-1.190542	-2.164039	-0.146704
Core RigidRotor			
SymmetryFactor 1			
End			
Tunneling Eckart			

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        ImaginaryFrequency[1/cm]      1091.8980
        WellDepth[kcal/mol]           6.4
        WellDepth[kcal/mol]           26.8
    End
    Frequencies[1/cm]      32
292.5064      390.5969
445.6905      490.1446      610.5368
612.8834      690.7877      739.6811
852.0582      897.3893      982.0545
986.3744      1000.2288      1012.3582
1051.1442      1054.0477      1061.0841
1162.2230      1185.5597      1196.6728
1342.3290      1359.6234      1488.5663
1501.0582      1625.1997      1645.5901
3192.6597      3200.7358      3202.7108
3216.0578      3218.9384      3226.4641
        ZeroEnergy[kcal/mol]          29.8
        ElectronicLevels[1/cm]        1
            0      2
    End
Barrier      B5      W1      W4      #      ts5
    RRHO
        Geometry[angstrom]      13
C      1.469203      0.728295      -0.032606
C      1.469196      -0.728303      -0.032703
C      0.170576      -1.178241      0.015685
C      -0.702276      0.000008      0.043888
C      0.170591      1.178246      0.015842
C      -2.171558      0.000013      -0.120714
H      2.359319      1.353445      -0.058722
H      2.359305      -1.353459      -0.058869
H      -0.175187      -2.208936      0.026277
H      -0.175157      2.208943      0.026530
H      -1.385264      -0.000122      1.067369
H      -2.708691      -0.942783      -0.169608
H      -2.708721      0.942806      -0.169329
    Core      RigidRotor
        SymmetryFactor      1
    End
    Tunneling      Eckart
        ImaginaryFrequency[1/cm]      1606.1738
        WellDepth[kcal/mol]           24.3
        WellDepth[kcal/mol]           52.8
    End
    Frequencies[1/cm]      32
225.3778      322.6284
403.6140      569.2739      590.8484
647.0042      656.4360      677.9656
756.5465      824.2011      861.5694
874.9567      910.2350      918.0160
1031.1063      1032.4404      1083.6221
1089.4348      1247.0402      1299.3931

```

1342.5482	1409.8071	1437.9732
1511.9528	1572.3716	2267.8317
3189.9641	3228.9935	3238.1829
3252.0729	3259.5272	3318.5981

ZeroEnergy[kcal/mol] 52.8

ElectronicLevels[1/cm] 1

0 2

End

Barrier B6 P1 W4 # ts6

Variational

RRHO

Geometry[angstrom] 13 #17

C	1.473971	0.738424	0.036497
C	1.473969	-0.738439	0.036469
C	0.184416	-1.180599	-0.030017
C	-0.688558	0.000004	-0.080570
C	0.184416	1.180575	-0.029902
C	-2.060324	0.000051	-0.138659
H	2.367538	1.358276	0.080280
H	2.367542	-1.358262	0.080471
H	-0.163312	-2.210530	-0.045124
H	-0.163187	2.210546	-0.045175
H	-2.609737	0.930374	-0.281726
H	-2.596275	-0.000377	1.730301
H	-2.609906	-0.930129	-0.281940

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 32

217.2730	330.1203	
393.0242	503.0630	538.7276
644.4773	686.3891	702.6889
782.0767	814.3409	848.2079
905.5477	909.5482	917.1907
969.2365	996.2510	1015.8088
1088.9878	1102.4619	1251.9544
1354.8767	1362.5049	1439.4926
1518.2952	1611.8914	1683.9524
3168.0172	3228.4646	3237.9415
3255.3990	3260.6176	3269.8887

ZeroEnergy[kcal/mol] 55.3

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #22

C	-1.472035	-0.738710	0.041210
C	-1.472093	0.738599	0.041193
C	-0.185032	1.181978	-0.033665
C	0.691844	0.000049	-0.088600
C	-0.184947	-1.181939	-0.033750
C	2.051401	0.000083	-0.154890

H	-2.365738	-1.357925	0.091986
H	-2.365824	1.357728	0.092380
H	0.161715	2.212248	-0.051690
H	0.162192	-2.212073	-0.051504
H	2.607801	-0.931187	-0.259919
H	2.616937	-0.000305	1.809615
H	2.608086	0.931153	-0.259856
Core RigidRotor			
SymmetryFactor 1			
End			
Frequencies[1/cm] 32			
200.9464	286.8333		
350.6233	391.4057	522.5000	
640.8987	679.7650	699.1939	
785.0952	820.3518	827.0046	
910.7671	913.6835	914.8147	
966.9527	989.9374	1013.7981	
1090.5820	1102.6631	1252.5453	
1358.4100	1370.9108	1445.1427	
1522.4311	1660.9816	1697.6724	
3168.5161	3227.8152	3237.3648	
3255.0920	3260.2241	3269.5560	
ZeroEnergy[kcal/mol]		55.6	
ElectronicLevels[1/cm]		1	
0	2		
End			
RRHO			
Geometry[angstrom] 13 #26			
C	-1.471236	-0.738721	0.045218
C	-1.471145	0.738821	0.045203
C	-0.185481	1.182725	-0.036330
C	0.693339	-0.000024	-0.094753
C	-0.185648	-1.182715	-0.036299
C	2.045714	-0.000090	-0.169381
H	-2.364967	-1.357487	0.101353
H	-2.364839	1.357673	0.101028
H	0.161170	2.213007	-0.056152
H	0.160706	-2.213094	-0.056278
H	2.605902	-0.931501	-0.251085
H	2.642904	0.000041	1.890069
H	2.605860	0.931386	-0.250882
Core RigidRotor			
SymmetryFactor 1			
End			
Frequencies[1/cm] 32			
180.8850	215.2908		
305.6596	345.4506	512.2685	
638.6655	678.9621	696.4352	
787.0547	816.5759	822.5424	
913.0188	913.7085	915.5596	
966.3737	988.7561	1012.6562	
1091.6798	1102.0603	1252.4802	

1360.4031	1373.3728	1449.0780
1524.6380	1695.3428	1710.0733
3168.4426	3227.3630	3237.0022
3254.8763	3259.9933	3268.0385

ZeroEnergy[kcal/mol] 55.4

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #29

C	-1.470897	-0.738697	0.049079
C	-1.470569	0.738974	0.049054
C	-0.185855	1.183238	-0.038658
C	0.693817	-0.000007	-0.100546
C	-0.186461	-1.183128	-0.038608
C	2.041984	-0.000303	-0.182293
H	-2.364534	-1.357177	0.109674
H	-2.364096	1.357706	0.108683
H	0.160793	2.213507	-0.060374
H	0.159277	-2.213686	-0.060859
H	2.603970	-0.931831	-0.249486
H	2.668481	-0.000340	1.972778
H	2.603992	0.931361	-0.248594

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 32

149.5539	155.8073	
254.5251	343.9459	505.3446
637.0537	679.5184	694.3043
787.6206	809.0857	822.1782
912.2395	914.3117	916.0240
966.0160	988.8150	1011.9696
1092.4523	1101.0246	1252.0209
1361.4937	1371.6649	1451.6660
1526.0943	1682.7714	1752.7920
3168.4991	3227.1882	3236.8204
3254.5960	3259.8359	3266.7809

ZeroEnergy[kcal/mol] 55.1

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #36

C	-1.470999	-0.738933	0.052440
C	-1.471019	0.738894	0.052441
C	-0.186629	1.183177	-0.040844
C	0.693725	0.000021	-0.105820
C	-0.186594	-1.183161	-0.040850
C	2.040393	0.000009	-0.193889
H	-2.364296	-1.357564	0.117373
H	-2.364328	1.357499	0.117427

H	0.159106	2.213748	-0.064580
H	0.159234	-2.213701	-0.064554
H	2.603151	-0.931780	-0.252474
H	2.690668	-0.000007	2.058405
H	2.603204	0.931764	-0.252469
Core RigidRotor			
SymmetryFactor 1			
End			
Frequencies[1/cm] 32			
112.2302	113.2493		
232.7285	343.6481	500.9557	
636.0752	680.0739	692.4326	
787.4204	802.1676	820.7693	
912.0052	914.2423	915.7030	
965.6197	988.5528	1011.4951	
1092.7857	1099.7893	1251.4898	
1361.7754	1368.4873	1452.8576	
1525.3004	1666.2392	1778.7565	
3168.0989	3226.6435	3236.3061	
3254.0095	3259.3295	3265.5911	
ZeroEnergy[kcal/mol]		54.7	
ElectronicLevels[1/cm]		1	
0	2		
End			
RRHO			
Geometry[angstrom] 13 #41			
C	-1.470978	-0.739036	0.055489
C	-1.471097	0.738855	0.055615
C	-0.186985	1.183169	-0.042771
C	0.693353	0.000097	-0.110885
C	-0.186793	-1.183123	-0.042980
C	2.039388	0.000204	-0.204877
H	-2.363955	-1.357756	0.124066
H	-2.364173	1.357418	0.124312
H	0.158517	2.213801	-0.068027
H	0.158895	-2.213689	-0.068375
H	2.602677	-0.931619	-0.258472
H	2.704159	-0.001263	2.147275
H	2.602549	0.932114	-0.258328
Core RigidRotor			
SymmetryFactor 1			
End			
Frequencies[1/cm] 32			
80.8857	160.8325		
223.4825	343.1941	497.3569	
635.1966	680.4621	690.6474	
786.6302	795.2591	818.5004	
911.7045	913.6938	914.9675	
965.0096	986.6748	1011.2424	
1092.7801	1098.3990	1250.7439	
1361.7718	1363.4772	1453.4235	
1524.7933	1648.7160	1788.6616	

3167.7800	3226.4526	3236.0975
3253.6692	3259.1080	3264.8316

ZeroEnergy[kcal/mol] 54.6

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #47

C	-1.470854	-0.739010	0.058181
C	-1.470906	0.738928	0.058241
C	-0.186921	1.183068	-0.044857
C	0.693027	0.000041	-0.115754
C	-0.186839	-1.183045	-0.044952
C	2.039051	0.000094	-0.215126
H	-2.363565	-1.357745	0.130115
H	-2.363657	1.357594	0.130249
H	0.158457	2.213722	-0.071555
H	0.158631	-2.213665	-0.071730
H	2.602466	-0.931855	-0.265879
H	2.705906	-0.000584	2.240216
H	2.602412	0.932077	-0.265813

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 32

58.4059	211.8244	
227.2860	342.8137	494.4845
634.5267	680.3529	688.9578
785.6719	788.8966	815.9233
911.5202	912.9650	914.1061
964.3469	983.4730	1011.0538
1092.4539	1097.0154	1249.9259
1357.9619	1361.5341	1453.4079
1524.0762	1632.9906	1783.5988
3167.3038	3226.3310	3235.9406
3253.3783	3258.9295	3264.3477

ZeroEnergy[kcal/mol] 54.3

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #52

C	-1.470255	-0.739016	0.060064
C	-1.470287	0.738958	0.060085
C	-0.186400	1.182962	-0.047072
C	0.693137	0.000030	-0.120427
C	-0.186349	-1.182941	-0.047123
C	2.039425	0.000036	-0.224287
H	-2.362690	-1.357814	0.134878
H	-2.362746	1.357708	0.134974
H	0.158831	2.213645	-0.075030
H	0.159004	-2.213583	-0.075016

H	2.602857	-0.932023	-0.273474
H	2.686227	-0.000191	2.339676
H	2.602887	0.932076	-0.273443
Core RigidRotor			
SymmetryFactor 1			
End			
Frequencies[1/cm] 32			
43.4524	211.6311		
231.6594	342.5336		492.2934
634.0240	679.8323		687.4944
783.6889	784.7600		813.3835
911.3778	912.2494		913.2836
963.7155	980.0233		1010.8886
1091.9118	1095.7470		1249.1002
1352.6346	1361.1751		1453.0309
1523.3331	1620.1907		1768.8002
3166.6986	3226.2568		3235.8247
3253.1492	3258.7947		3263.9900
ZeroEnergy[kcal/mol]		54.1	
ElectronicLevels[1/cm]		1	
0	2		
End			
RRHO			
Geometry[angstrom] 13 #58			
C	-1.468792	-0.739035	0.060350
C	-1.468844	0.738963	0.060447
C	-0.185024	1.182867	-0.049570
C	0.694213	0.000038	-0.124688
C	-0.184941	-1.182853	-0.049715
C	2.040858	0.000130	-0.231475
H	-2.361030	-1.357874	0.137145
H	-2.361129	1.357732	0.137289
H	0.160232	2.213526	-0.078204
H	0.160320	-2.213505	-0.078558
H	2.604371	-0.931960	-0.279561
H	2.628200	-0.000896	2.449223
H	2.604222	0.932318	-0.279430
Core RigidRotor			
SymmetryFactor 1			
End			
Frequencies[1/cm] 32			
33.4666	207.8159		
219.4899	342.3146		490.5212
633.6122	679.1113		686.2370
779.4586	783.9832		811.1135
911.2223	911.6618		912.5910
963.1682	976.5769		1010.7483
1091.2812	1094.6708		1248.3330
1347.9505	1360.7749		1452.4300
1522.7071	1610.4912		1750.0632
3166.1189	3226.2142		3235.7522
3253.0154	3258.7223		3263.7861

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ZeroEnergy[kcal/mol]          53.9
ElectronicLevels[1/cm]       1
    0    2
End
RRHO
Geometry[angstrom]          13 #65
C          -1.465615    -0.739159    0.057053
C          -1.465811     0.738864    0.057331
C          -0.181884     1.182824   -0.052737
C           0.697287     0.000174   -0.127800
C          -0.181570    -1.182736   -0.053179
C           2.044505     0.000352   -0.233977
H          -2.357743    -1.358154    0.133894
H          -2.358099     1.357600    0.134412
H           0.163188     2.213553   -0.081279
H           0.163794    -2.213356   -0.082116
H           2.608106    -0.931803   -0.280201
H           2.491385    -0.002397    2.574984
H           2.607903     0.932646   -0.279841
Core      RigidRotor
SymmetryFactor      1
End
Frequencies[1/cm]          32
23.8694          194.6711
212.0527          342.1686          489.1033
633.3029          678.3606          685.1871
776.1198          783.3321          809.2265
911.0282          911.3157          912.0479
962.6862          973.6160        1010.6184
1090.6511         1093.7989        1247.6708
1344.1623         1360.3785        1451.6999
1522.1377         1603.2716        1731.2402
3165.5701         3226.1874        3235.6904
3252.8976         3258.6539        3263.6259
ZeroEnergy[kcal/mol]          53.7
ElectronicLevels[1/cm]       1
    0    2
End
End
Barrier      B7      W6      W5      #      ts7
RRHO
Geometry[angstrom]          13
C           1.415694     0.775273   -0.016049
C           0.080086     1.161466   -0.012519
C          -0.780281     0.010227   -0.022315
C           0.074814    -1.138881   -0.047726
C           1.480103    -0.651441   -0.031801
C          -2.189629    -0.001570    0.007728
H           2.279512     1.432994    0.030209
H          -0.278448     2.187367    0.052867
H           0.877108    -1.083066    1.023391
H          -0.213688    -2.177814   -0.183815

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H	2.347988	-1.281208	-0.208100
H	-2.744163	-0.937588	0.013155
H	-2.753027	0.928877	0.008387
Core RigidRotor			
	SymmetryFactor	0.5	
End			
Tunneling Eckart			
	ImaginaryFrequency[1/cm]	1336.1277	
	WellDepth[kcal/mol]	28.8	
	WellDepth[kcal/mol]	34.1	
End			
	Frequencies[1/cm]	32	
255.4312	338.8706		
449.4623	585.3164	605.6124	
661.2246	665.8588	745.2110	
766.9402	839.5208	892.7490	
934.5180	954.6778	960.1138	
1009.6424	1075.1586	1082.3079	
1221.6471	1238.3536	1276.5358	
1367.1599	1414.9659	1463.1336	
1490.5630	1512.5295	2133.6626	
3179.9573	3229.6426	3247.5949	
3255.1207	3266.0571	3286.1778	
	ZeroEnergy[kcal/mol]	41.5	
	ElectronicLevels[1/cm]	1	
	0 2		
End			
Barrier	B8	W1	W5 # ts8
RRHO			
	Geometry[angstrom]	13	
C	1.437807	0.736106	-0.055870
C	0.122232	1.171938	0.039023
C	-0.752201	0.020300	0.079574
C	0.164651	-1.168898	-0.001526
C	1.477043	-0.686836	-0.072691
C	-2.179530	0.008719	-0.111714
H	2.314598	1.381181	-0.057197
H	-0.223266	2.201271	0.093049
H	-0.430140	-0.591668	1.136565
H	-0.190812	-2.195106	-0.049614
H	2.371905	-1.303794	-0.081853
H	-2.734514	-0.925875	-0.146756
H	-2.727790	0.946020	-0.154972
Core RigidRotor			
	SymmetryFactor	0.5	
End			
Tunneling Eckart			
	ImaginaryFrequency[1/cm]	1218.1417	
	WellDepth[kcal/mol]	17.7	
	WellDepth[kcal/mol]	38.6	
End			
	Frequencies[1/cm]	32	

272.1545	318.9849	
327.1723	544.0305	586.0819
635.7734	681.1462	749.2641
758.6280	841.2369	871.6481
907.4219	914.2290	955.1477
1068.6832	1079.9434	1083.9856
1142.9747	1244.6564	1310.3674
1324.2400	1449.4184	1460.9922
1494.5406	1520.6464	2046.9224
3185.8628	3228.7276	3245.3987
3253.7859	3263.8760	3299.8961

ZeroEnergy[kcal/mol] 46.0

ElectronicLevels[1/cm] 1

0 2

End

Barrier B9 P1 W5 # ts9

Variational

RRHO

Geometry[angstrom] 13 #96

C	1.504259	-0.616636	-0.036728
C	1.433447	0.758581	-0.002395
C	0.074666	1.184379	0.027184
C	-0.785552	0.040562	0.002990
C	0.117930	-1.180740	-0.009584
C	-2.150741	0.029543	-0.024951
H	2.411925	-1.214945	-0.064219
H	2.291902	1.429061	0.001733
H	-0.267769	2.216897	0.054918
H	-0.111002	-1.908082	-0.798606
H	-2.711660	-0.903856	-0.044470
H	-2.717122	0.960058	-0.023430
H	-0.060324	-1.873264	1.134981

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 32

353.6791	484.6481	
570.0078	624.1141	636.2194
678.1272	766.4498	817.9614
847.1921	856.6355	910.0652
935.2677	959.7869	991.1267
1032.1827	1105.1220	1173.2048
1195.3180	1262.9820	1297.5573
1331.4158	1393.8804	1426.2192
1435.2050	1514.4277	1588.4052
3116.1195	3169.2602	3222.6858
3240.0898	3254.4204	3268.9717

ZeroEnergy[kcal/mol] 20.0

ElectronicLevels[1/cm] 1

0 2

End

RRHO

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      Geometry[angstrom]      13 #92
C           1.501148      -0.618731      -0.053947
C           1.432804       0.758653      -0.004162
C           0.077087       1.186009       0.039817
C          -0.785669       0.041427       0.004753
C           0.118555      -1.175305      -0.013305
C          -2.149263       0.030712      -0.036667
H           2.406716      -1.219113      -0.094751
H           2.292964       1.426825       0.001054
H          -0.264410       2.218301       0.080133
H          -0.129560      -1.946595      -0.750390
H          -2.709754      -0.902654      -0.065879
H          -2.715487       0.961297      -0.034504
H          -0.048439      -1.874650       1.245401

      Core      RigidRotor
      SymmetryFactor      0.5
End
      Frequencies[1/cm]      32
349.3701           389.3199
508.7581           587.1639           627.1595
641.7397           682.8550           764.3747
817.7388           853.5002           854.6986
930.8917           953.5279           985.0755
1004.4922          1031.9021          1109.4433
1154.1380          1255.5269          1289.1644
1309.8772          1354.9921          1397.7911
1426.2271          1507.3799          1595.5035
3139.3449          3169.8237          3223.8869
3241.7070          3256.2621          3269.6739

      ZeroEnergy[kcal/mol]      28.1
      ElectronicLevels[1/cm]      1
      0      2
End
      RRHO
      Geometry[angstrom]      13 #87
C           1.485045      -0.630096      -0.096142
C           1.427578       0.759078      -0.010758
C           0.089031       1.191934       0.070282
C          -0.784518       0.042222       0.011714
C           0.117093      -1.165641      -0.015834
C          -2.140186       0.035099      -0.066183
H           2.384964      -1.235021      -0.170666
H           2.294989       1.417648      -0.008180
H          -0.248898       2.223248       0.143159
H          -0.174638      -2.027282      -0.619484
H          -2.700724      -0.897379      -0.118945
H          -2.705655       0.966293      -0.066844
H          -0.014292      -1.843089       1.482482

      Core      RigidRotor
      SymmetryFactor      0.5
End
      Frequencies[1/cm]      32

```

225.8831	354.0920	
497.0767	583.5935	631.1365
639.6536	683.6986	762.2815
816.2089	850.4640	865.4426
928.2131	947.0167	969.2938
997.7847	1030.7680	1104.3449
1114.0330	1245.0354	1275.8497
1290.1008	1302.7312	1397.3901
1428.6720	1496.9209	1610.3474
3161.5727	3170.2773	3225.1369
3243.7424	3258.2920	3270.1041

ZeroEnergy[kcal/mol] 36.6

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #83

C	1.485045	-0.630096	-0.096142
C	1.427578	0.759078	-0.010758
C	0.089031	1.191934	0.070282
C	-0.784518	0.042222	0.011714
C	0.117093	-1.165641	-0.015834
C	-2.140186	0.035099	-0.066183
H	2.384964	-1.235021	-0.170666
H	2.294989	1.417648	-0.008180
H	-0.248898	2.223248	0.143159
H	-0.174638	-2.027282	-0.619484
H	-2.700724	-0.897379	-0.118945
H	-2.705655	0.966293	-0.066844
H	-0.014292	-1.843089	1.482482

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 32

223.5300	352.9861	
495.0658	584.9470	637.2866
646.7316	685.7957	762.4277
811.1726	842.9150	887.0044
923.9921	932.0071	963.5211
993.0819	1030.1670	1056.9617
1099.6214	1199.8081	1242.4090
1274.4107	1305.9391	1398.7611
1434.3731	1482.8616	1643.9410
3170.0283	3187.3302	3226.3323
3246.3932	3260.0022	3269.5032

ZeroEnergy[kcal/mol] 45.0

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #77

C	1.455874	-0.651875	-0.129999
---	----------	-----------	-----------

C	1.417518	0.763903	-0.015882
C	0.106325	1.200024	0.088333
C	-0.778687	0.039569	0.015791
C	0.117141	-1.162649	-0.009369
C	-2.125351	0.040453	-0.089083
H	2.351240	-1.258143	-0.241301
H	2.295801	1.407627	-0.015578
H	-0.230637	2.228852	0.190820
H	-0.205704	-2.094966	-0.471205
H	-2.689085	-0.889474	-0.158029
H	-2.687075	0.974193	-0.100455
H	0.008541	-1.744643	1.637006
Core RigidRotor			
SymmetryFactor 0.5			
End			
Frequencies[1/cm] 32			
221.2527	349.5487		
490.6403	577.3177	655.3423	
665.7600	703.4842	773.6546	
791.5030	819.3215	877.8196	
921.9253	928.7648	939.5825	
963.7556	1028.5798	1052.2241	
1076.3928	1098.9331	1246.0961	
1302.7258	1326.4616	1390.5811	
1456.6848	1490.9891	1724.3604	
3169.5201	3217.7650	3228.4905	
3250.0702	3259.7462	3267.7002	
ZeroEnergy[kcal/mol]		52.4	
ElectronicLevels[1/cm]		1	
0	2		
End			
RRHO			
Geometry[angstrom] 13 #77			
C	1.455874	-0.651875	-0.129999
C	1.417518	0.763903	-0.015882
C	0.106325	1.200024	0.088333
C	-0.778687	0.039569	0.015791
C	0.117141	-1.162649	-0.009369
C	-2.125351	0.040453	-0.089083
H	2.351240	-1.258143	-0.241301
H	2.295801	1.407627	-0.015578
H	-0.230637	2.228852	0.190820
H	-0.205704	-2.094966	-0.471205
H	-2.689085	-0.889474	-0.158029
H	-2.687075	0.974193	-0.100455
H	0.008541	-1.744643	1.637006
Core RigidRotor			
SymmetryFactor 0.5			
End			
Frequencies[1/cm] 32			
221.2527	349.5487		
490.6403	577.3177	655.3423	

665.7600	703.4842	773.6546
791.5030	819.3215	877.8196
921.9253	928.7648	939.5825
963.7556	1028.5798	1052.2241
1076.3928	1098.9331	1246.0961
1302.7258	1326.4616	1390.5811
1456.6848	1490.9891	1724.3604
3169.5201	3217.7650	3228.4905
3250.0702	3259.7462	3267.7002

ZeroEnergy[kcal/mol] 52.4

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #66

C	1.419221	-0.687860	-0.129528
C	1.410990	0.772141	-0.000169
C	0.123614	1.210099	0.072694
C	-0.763126	0.038361	-0.011410
C	0.122785	-1.150605	-0.067700
C	-2.112061	0.043861	-0.078213
H	2.313140	-1.299627	-0.230763
H	2.303752	1.394147	0.029148
H	-0.218693	2.236802	0.177723
H	-0.219228	-2.156428	-0.297049
H	-2.678617	-0.884875	-0.145956
H	-2.673298	0.978226	-0.063992
H	-0.035590	-1.624228	1.816842

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 32

209.8018	339.3715	
366.4356	437.2038	503.6812
650.4949	679.9865	720.6211
788.9620	797.0284	824.5079
912.5280	932.1055	936.2067
965.8318	970.8153	1021.2407
1084.7177	1101.7864	1252.5648
1366.2528	1371.1311	1440.7634
1482.1978	1633.4961	1713.0942
3167.7364	3230.1976	3241.1039
3255.0479	3260.9973	3266.9715

ZeroEnergy[kcal/mol] 58.0

ElectronicLevels[1/cm] 1

0 2

End

RRHO

Geometry[angstrom] 13 #61

C	1.413850	-0.695249	-0.122814
C	1.411248	0.772450	0.006706
C	0.125831	1.212070	0.064686

C	-0.759650	0.039167	-0.025954
C	0.123713	-1.147074	-0.096116
C	-2.110048	0.043630	-0.069315
H	2.308247	-1.309484	-0.206051
H	2.306410	1.390312	0.046934
H	-0.217583	2.238887	0.164680
H	-0.220974	-2.162842	-0.270808
H	-2.676319	-0.885298	-0.138095
H	-2.672654	0.976751	-0.034840
H	-0.056790	-1.598295	1.895024
Core RigidRotor			
SymmetryFactor 0.5			
End			
Frequencies[1/cm] 32			
194.6872	261.6550		
309.7939	342.0978	495.6232	
648.8130	681.2430	715.9837	
787.9567	795.0414	824.0116	
912.8587	931.3008	934.5807	
966.0210	975.3687	1017.1300	
1091.9693	1102.4402	1252.7100	
1364.0557	1372.4836	1453.6606	
1542.3979	1663.4915	1701.1469	
3167.0387	3229.6596	3239.8704	
3256.0084	3261.8469	3266.4939	
ZeroEnergy[kcal/mol]		57.6	
ElectronicLevels[1/cm]		1	
0	2		
End			
RRHO			
Geometry[angstrom] 13 #56			
C	1.411415	-0.699437	-0.118892
C	1.411784	0.771690	0.010811
C	0.126647	1.212787	0.058913
C	-0.758004	0.039285	-0.037302
C	0.123797	-1.145169	-0.117153
C	-2.109147	0.042622	-0.063364
H	2.305999	-1.315335	-0.188740
H	2.308085	1.387358	0.058434
H	-0.217265	2.239755	0.155503
H	-0.222469	-2.165474	-0.258970
H	-2.675077	-0.886417	-0.134240
H	-2.672581	0.974557	-0.012561
H	-0.065643	-1.565109	1.982490
Core RigidRotor			
SymmetryFactor 0.5			
End			
Frequencies[1/cm] 32			
153.5739	204.5343		
239.7358	341.0433	492.1127	
646.8195	682.1227	711.3252	
783.9411	794.1617	821.4210	

913.0304	929.3196	933.2606
965.6089	976.9320	1015.7767
1095.8550	1101.8192	1252.1263
1362.4916	1369.1180	1456.2935
1599.1147	1665.3075	1698.5387
3166.5562	3229.0747	3238.9953
3256.2762	3262.5601	3266.0365

ZeroEnergy[kcal/mol] 57.1

ElectronicLevels[1/cm] 1

0 2

End

End

Barrier B10 P1 W6 # ts10

RRHO

Geometry[angstrom] 13

C	1.334491	0.815986	-0.073929
C	0.032740	1.203587	-0.004181
C	-0.804822	-0.008571	-0.009770
C	0.116052	-1.154512	-0.105339
C	1.393325	-0.667626	-0.116131
C	-2.152694	-0.062041	0.054857
H	2.206610	1.466663	-0.080001
H	-0.350811	2.219237	0.056260
H	-0.192671	-2.196012	-0.148542
H	2.299247	-1.245785	-0.284259
H	1.956769	-0.836491	1.821057
H	-2.681842	-1.015115	0.045597
H	-2.751853	0.846561	0.116847

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 763.9084

WellDepth[kcal/mol] 3.1

WellDepth[kcal/mol] 45.2

End

Frequencies[1/cm] 32

188.5327	260.4616	
310.3258	342.9634	513.6027
637.5472	678.1693	687.3819
779.5420	806.8728	810.4620
912.3103	917.6278	942.2846
964.3111	978.4739	1007.0325
1091.1329	1094.9774	1249.6046
1347.6958	1360.3115	1461.6972
1547.5599	1595.2278	1777.6398
3168.1646	3231.6050	3239.7301
3255.2676	3261.4119	3266.0496

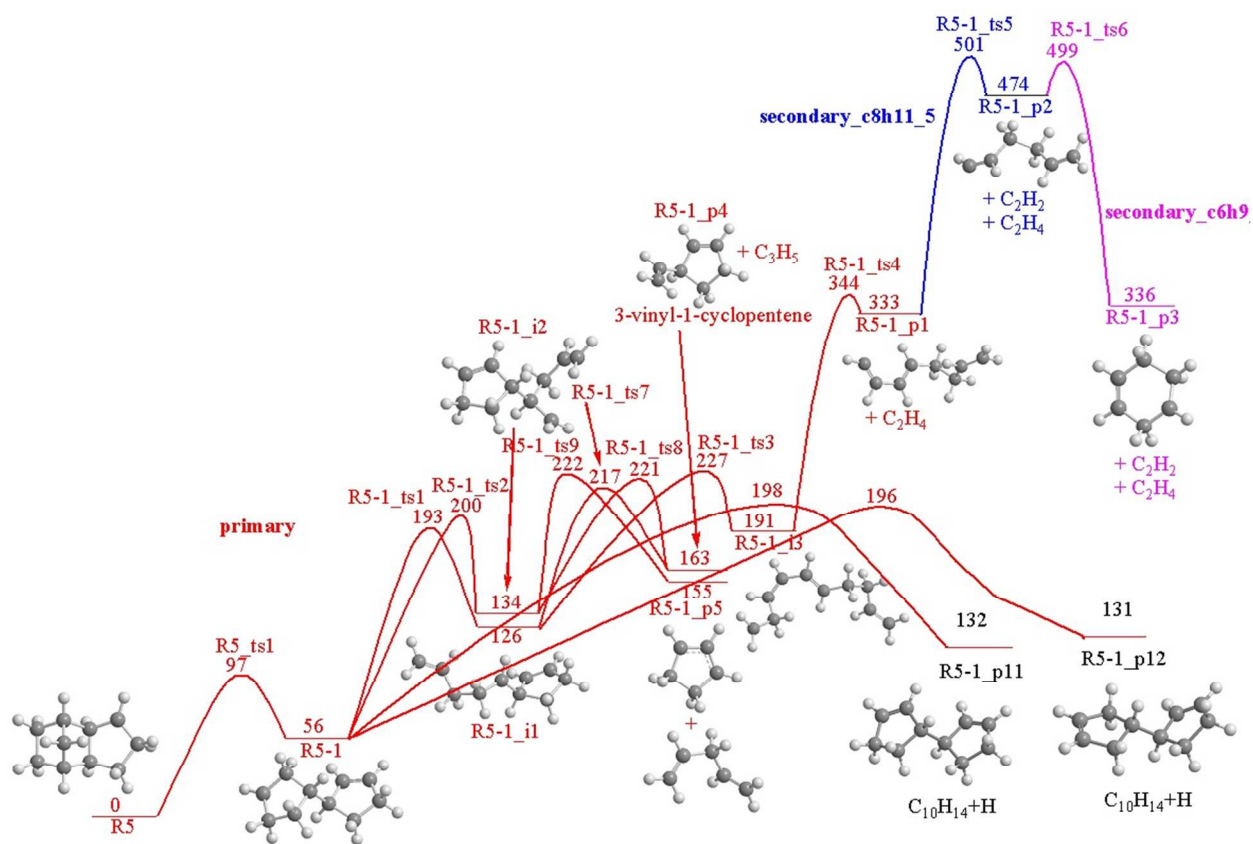
ZeroEnergy[kcal/mol] 57.9

ElectronicLevels[1/cm] 1

0 2

Cartesian coordinates and vibrational frequencies of stationary points in R5 channel

Please refer to the following schemes for the notation of stationary points involved in R5 channel. Cartesian coordinates and vibrational frequencies of the stationary points are given below in the form of the corresponding fragments of the MESS input file.



Scheme S5. R5 channel.

R5_primary

```
!-----c10h15_R5-1-----
Well      R5-1
Species
RRHO
Geometry[angstrom]  25
C   -0.6849727808   -2.3405431737   2.6437116761
C    0.5493772188   -2.0587098816   1.7539107275
```

C	0.2653607064	-0.690907247	1.0828147604
C	-0.5800808354	-0.8308333614	-0.2123495595
C	-0.942676674	0.5069183325	-0.8287026667
C	-1.1961623094	-0.9749295557	2.9777441438
C	-0.4711289951	0.0847971535	2.2099272336
C	0.1831998324	-1.5307628001	-1.3799823033
C	-0.3081670764	0.7378061922	-1.9760169599
C	0.5849923952	-0.4106442829	-2.3752222664
H	-0.4320254207	-2.9359491304	3.5303252478
H	-1.4381464814	-2.932488203	2.0988514115
H	0.7439345678	-2.8572162695	1.0350286792
H	1.438914935	-1.9700796033	2.3857607108
H	1.1997234478	-0.1866622511	0.8150011818
H	-1.4876695807	-1.3928990299	0.0409264801
H	-1.626206092	1.2030580938	-0.3567824328
H	-1.9698071575	-0.7755991045	3.7087353258
H	-1.1285549396	0.876501807	1.8361042671
H	0.2698575396	0.5980951062	2.8468348228
H	-0.4847454246	-2.2372445309	-1.8790153823
H	1.046609086	-2.1007647423	-1.0313002312
H	-0.3929160453	1.647552138	-2.5603781176
H	0.4379850056	-0.7138753954	-3.4169933667
H	1.6429110788	-0.1321022605	-2.2850013819

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 69

59.4423	70.5325	116.0057
154.6075	212.9441	271.3873
325.4994	351.3083	394.8131
475.0530	642.3430	682.0170
690.6067	740.5767	791.6148
803.8485	825.1432	871.0682
894.9651	903.4751	915.1333
920.3805	934.9358	960.9819
977.2848	998.2422	1006.0051
1043.3642	1049.1117	1059.7782
1075.7569	1133.5784	1137.8986
1151.0974	1189.1977	1216.2000
1238.8204	1252.9254	1270.6476
1286.2373	1303.6777	1317.0321
1320.2391	1327.4570	1344.9652
1365.1455	1378.2675	1386.2748
1472.3011	1475.2528	1486.1232
1500.3858	1505.6686	1681.2643
2923.3046	2942.4346	3001.0109
3002.2865	3003.6680	3029.3266
3036.8561	3038.2166	3043.7574
3053.9736	3083.6339	3091.7294
3165.3080	3189.2106	3191.2469

ZeroEnergy[kcal/mol] 13.38

ElectronicLevels[1/cm] 1

```

0 2
End
End
!-----
!-----c10h15_R5-1_i1-----
Well      R5-1_i1
Species
RRHO
Geometry[angstrom] 25
C  -0.5271358955  -1.1066509472  2.6518883939
C  0.71582079    -1.236539176   1.7169063674
C  0.7463545525  -0.2693374718   0.5787902636
C  0.0566461987  -0.5327966165   -0.7259217784
C  -0.6303874422  0.7096619361   -1.2691352345
C  -0.5801683305  0.1950262905   3.3979112035
C  -0.5813052456  0.3170166041   4.7224251431
C  1.0300461517  -0.9015323578   -1.9073647089
C  -0.0163392315  1.211913192    -2.3384864512
C  1.1785189352  0.3869630877   -2.7541747056
H  -0.5240764918  -1.9393714596   3.3631337004
H  -1.4305030404  -1.2146982561   2.0381143169
H  0.7201093707   -2.2633413425   1.3270009547
H  1.6137766095   -1.1251304753   2.3337237561
H  1.3064947735   0.6558960713    0.6768828979
H  -0.6615315652  -1.3488777978   -0.5775875282
H  -1.4893770848  1.1509980866   -0.7763118033
H  -0.6103839418  1.0939653802   2.7846820959
H  -0.616466612   1.2871730095   5.2056299492
H  -0.5507697948  -0.5517194876   5.3740061191
H  0.5658673321   -1.685183793    -2.5121682222
H  1.9851256519   -1.286438553    -1.5458414527
H  -0.3068268376  2.1227865686   -2.8503735768
H  1.190402179    0.1737356175   -3.8279239645
H  2.1124609691   0.9208728899   -2.5365377354
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
20.2584          28.3166          66.9526
89.3765          120.1051         180.8690
252.3137         314.8593         334.5788
384.7673         439.8902         468.6223
540.2853         666.0116         688.6645
722.1915         779.9868         790.0957
825.7281         854.9957         888.2569
915.2544         942.4169         949.9831
967.7119         972.3031         981.0338
1023.4035        1027.2517        1039.4573
1076.8915        1107.8801        1125.9421
1134.1984        1175.4730        1203.6266
1218.3775        1254.1019        1265.9307
1293.7462        1310.0594        1318.2148

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1321.4981      1332.7353      1355.2460
1370.4967      1409.9931      1452.9845
1482.9788      1484.1935      1486.3001
1500.8115      1673.7983      1705.7942
2990.2903      3002.7264      3004.5647
3005.7466      3037.5401      3044.6090
3052.2019      3054.9331      3093.9075
3119.5501      3127.2800      3151.7579
3165.4015      3190.6645      3205.2556
ZeroEnergy[kcal/mol] 30.11
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R5-1_i3-----
Well      R5-1_i3
Species
RRHO
Geometry[angstrom] 25
C -1.1381222045 -0.7010745336 2.1856307376
C -0.6138264533 -1.4389022381 0.9245790686
C -0.6070406599 -0.6041383034 -0.3240852839
C -1.3851240602 -0.8320309786 -1.3910591676
C -1.441485108 -0.0584884315 -2.6347457605
C -0.3166085247 0.491590174 2.5884378517
C 0.3946939302 0.5826929526 3.7087876439
C 1.8936209383 0.3251286028 -4.1938456821
C -0.4404774105 0.5270599852 -3.3096753325
C 1.0311630383 0.5055557056 -2.9880805842
H -1.1723177068 -1.4137347252 3.0160410194
H -2.1698257172 -0.383942536 1.9904317017
H -1.2285369999 -2.3299970635 0.761909651
H 0.4046720103 -1.7878347531 1.1362567972
H 0.0591035391 0.254389165 -0.3295840168
H -2.0908762891 -1.6613149783 -1.3335605344
H -2.4337873521 0.0118987168 -3.0766466941
H -0.315725194 1.3331334033 1.8982776781
H 0.9729445294 1.4684955973 3.9470378651
H 0.4204284475 -0.2264805675 4.4330933492
H 2.9279112506 0.646359746 -4.1881173365
H 1.5445998687 -0.2571051305 -5.0382732323
H -0.6999503313 1.0591158789 -4.2223022818
H 1.3162448374 1.4373880449 -2.4772570994
H 1.2301146215 -0.2900287333 -2.2519813571
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
28.2926      52.9764      66.1073
98.9836      101.1181      133.2762
146.9568      157.9205      267.4880

```

283.6571	323.5058	384.0960
443.7001	453.5499	482.4741
526.9339	666.4768	705.8662
725.4485	792.3597	815.3108
868.3673	873.1999	946.1435
957.5745	982.1414	990.0738
1005.8033	1008.2220	1031.3462
1044.0640	1075.5804	1089.8279
1105.3239	1132.2735	1196.2298
1211.8561	1262.9174	1279.2514
1320.1069	1325.3325	1329.0704
1343.1636	1348.2858	1377.9287
1437.5726	1452.1224	1452.9479
1460.6884	1484.5956	1487.6925
1683.0630	1703.1186	1705.8538
2951.2853	2979.6566	3005.7406
3011.5395	3054.8274	3057.9888
3098.3377	3115.5640	3120.3888
3128.6375	3134.3307	3139.5104
3146.9856	3206.4764	3239.2542

ZeroEnergy[kcal/mol] 45.65

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h15_R5-1_i2-----

Well R5-1_i2

Species

RRHO

Geometry[angstrom] 25

C	-1.6232805452	-1.3226727798	2.7735769318
C	1.3164371858	-1.4983333926	1.4055133341
C	0.6547335849	-0.2454836741	0.9340805489
C	-0.2728609217	-0.4941677995	-0.2941306952
C	-1.0158361832	0.7486241393	-0.7418144344
C	-1.1859812015	-0.0668336097	2.8123720287
C	-0.0067096253	0.5401137738	2.094149208
C	0.5253422544	-0.8789215729	-1.5779595807
C	-0.5613802287	1.2321394782	-1.896280172
C	0.5583707247	0.3939462503	-2.4642392415
H	-2.4817330864	-1.6309751445	3.3604908284
H	-1.1415870214	-2.0869960018	2.1748390934
H	1.4037731238	-2.3686697969	0.7668887247
H	1.8221318307	-1.523882398	2.3638850196
H	1.4454118315	0.4370250525	0.5680576439
H	-0.9777376758	-1.2871566868	-0.0289495398
H	-1.81552026	1.1901259092	-0.1586396293
H	-1.7173715994	0.6360166685	3.4536601032
H	-0.3045307424	1.5256859283	1.7186807444
H	0.7694684266	0.7520487019	2.8432546398
H	-0.0034057517	-1.6746843929	-2.1084831842

```

H  1.5254516126   -1.2539956034   -1.3503671027
H  -0.9279578897    2.1302222398   -2.3814651062
H   0.4122136991    0.1610788866   -3.5239621988
H   1.5168154581    0.9247848247   -2.3979539642
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
54.2073              73.9769              108.1546
114.8559             126.7131             191.4099
214.3394             274.8688             345.6101
380.2411             383.9154             482.7115
491.5823             560.5875             663.8425
677.7854             742.3989             789.2553
804.5039             827.9021             884.7718
913.6450             921.3492             941.0446
945.5372             950.8259             982.3597
995.8875             1037.8170            1041.4032
1049.6840            1086.4013            1109.7717
1131.9163            1139.8869            1178.8878
1222.7541            1238.6850            1258.3511
1292.0357            1295.0177            1316.2525
1326.8702            1339.7467            1362.2583
1379.7888            1390.0431            1449.8964
1459.1305            1481.0244            1486.8946
1504.8742            1679.6960            1706.2853
2884.1204            2992.1449            3003.6222
3033.1169            3036.6017            3044.9304
3056.5613            3088.5942            3106.9180
3133.8786            3134.4581            3165.7155
3192.0634            3214.0042            3234.5155
ZeroEnergy[kcal/mol] 32.03
ElectronicLevels[1/cm] 1
0  2
End
End
!-----
!-----c3h5_c7h10_R5-1_p4-----
Bimolecular  R5-1_p4
Fragment      c7h10
RRHO
Geometry[angstrom]  17
C  1.1817730139   -0.7724252349    1.8596161019
C  -0.0117935235   -0.3950304035    1.4118243284
C  -0.545725589    -0.478998936    -0.0038519624
C  -0.853981487     0.9186722059   -0.5274136285
C   0.4158510824   -1.0286749281   -1.0912991805
C  -0.0168043336    1.290413205    -1.4924996566
C   0.9903693986    0.213020722    -1.8181267166
H   1.9345693827   -1.2171084034    1.2185418166
H   1.4511460537   -0.6466300864    2.9023255692
H   -0.7107734077    0.0454974465    2.1222556688

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H  -1.4633122556   -1.0813003274    0.0363651493
H  -1.6358419461    1.5375475085   -0.1013862595
H  -0.1692574445   -1.6184770254    -1.8012505266
H   1.1877783406   -1.6868395719   -0.6914683855
H  -0.0180857259    2.2612205547   -1.9755043058
H   1.1017202848    0.0462961984   -2.8941074302
H   1.9833161562    0.491182076   -1.4418425819
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  45
78.7618              104.4703              252.2270
309.6783              442.9227              504.0393
611.2926              698.9008              725.2028
789.8251              813.4693              881.9659
916.7422              937.0680              951.1960
972.0472              987.8899             1018.7914
1037.7857             1060.7625             1113.8057
1137.9979             1176.6010             1220.1023
1270.3017             1305.1428             1316.2123
1333.1565             1355.6650             1373.3659
1446.6832             1485.8491             1508.4461
1678.3216             1703.7056             2989.7210
3004.9072             3043.0389             3060.5853
3102.0922             3110.2345             3138.1389
3165.8185             3190.9018             3213.0619
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0  1
End
Fragment              c3h5
RRHO
Geometry[angstrom]    8
C  0.0  0.0  0.4414918248
H  0.0  0.0  1.5297451707
C  0.0  1.2274571769   -0.1957824309
C  0.0  -1.2274571769   -0.1957824309
H  0.0  2.1546553362    0.3627527557
H  0.0  -2.1546553362    0.3627527557
H  0.0  1.2960812234   -1.2782433226
H  0.0  -1.2960812234   -1.2782433226
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  18
429.8649              531.6773              551.3484
785.3716              810.5065              936.5863
1012.9503             1037.0010             1207.5850
1270.2294             1423.3954             1511.2262
1517.2794             3126.8472             3133.4950
3139.8670             3231.6020             3234.4382
ZeroEnergy[kcal/mol]    0.0

```

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ElectronicLevels[1/cm]      1
0  2
End
GroundEnergy[kcal/mol] 38.96
End
!-----c2h4_c8h11_R5-1_p1-----
Bimolecular      R5-1_p1
Fragment          c8h11
RRHO
Geometry[angstrom]      19
C  -0.323117088  -0.5149019236  1.9051916205
C  0.4717952748  -1.1859264913  0.768505337
C  0.302860528  -0.6309324023  -0.6193094596
C  -0.5886968139  0.2792607653  -1.0282911659
C  -0.727316879  0.7739132959  -2.4079475089
C  0.1921528488  0.8464722357  2.2876275909
C  0.5957388784  1.1872480135  3.5081465864
C  0.0961097185  0.598937927  -3.4185336283
H  -0.29345522  -1.1656871651  2.7843338325
H  -1.3783629502  -0.4456161913  1.6116687564
H  0.207987864  -2.2524685511  0.7361948663
H  1.5394134239  -1.1673868769  1.0235321128
H  0.977081346  -1.0495072496  -1.3648617099
H  -1.2921281785  0.7029298587  -0.317856122
H  -1.6306174359  1.3665824464  -2.5980747051
H  0.2418684076  1.5860123872  1.4917273541
H  0.9635865422  2.1831320638  3.7286754776
H  0.5707711056  0.4823072616  4.3343938483
H  0.1504736277  0.8803295963  -4.4588160831
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  51
30.3706  77.4815  86.0227
137.8803  172.4420  228.7291
236.2188  312.0682  421.0179
513.4516  592.2379  611.8730
664.5305  757.0350  829.7853
833.5152  876.7502  898.9047
934.0743  945.6712  999.4467
1010.8056  1031.3179  1045.0891
1089.3077  1133.6919  1209.8485
1261.0430  1275.5954  1321.9032
1331.3120  1346.8696  1356.6942
1385.1815  1454.9145  1470.4480
1490.4103  1637.2641  1702.9434
1706.0890  2989.3485  3003.5570
3009.9512  3019.9080  3056.1913
3120.7352  3121.5548  3137.0958
3153.0624  3205.4412  3246.3464
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1

```

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0 2
End
Fragment          c2h4
RRHO
Geometry[angstrom] 6
C 0.0 0.6634900906 0.0
C 0.0 -0.6634900906 0.0
H 0.0 1.23462754 -0.9225248038
H 0.0 1.23462754 0.9225248038
H 0.0 -1.23462754 0.9225248038
H 0.0 -1.23462754 -0.9225248038
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm] 12
834.2929          972.9227          974.1218
1066.8559         1238.5875         1379.4650
1472.0483         1691.5384         3121.2072
3136.3255         3192.3844         3220.8390
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 79.59
End
!-----c5h7_c5h8_R5-1_p5-----
Bimolecular      R5-1_p5
Fragment          c5h8
RRHO
Geometry[angstrom] 13
C -0.9590582092 -2.1713837036 -0.1801722802
C 0.9590582092 2.1713837036 -0.1801722802
C -0.0018870018 1.2527832294 -0.174266712
C 0.0018870018 -1.2527832294 -0.174266712
C 0.0 0.0 0.6668893539
H 0.9025969729 3.0499984902 -0.812951267
H -0.9025969729 -3.0499984902 -0.812951267
H -0.8823486242 -0.008511337 1.3179629254
H 0.8823486242 0.008511337 1.3179629254
H -0.8644546075 1.3771991382 -0.8263379051
H 0.8644546075 -1.3771991382 -0.8263379051
H 1.8375352291 2.079945644 0.4520385619
H -1.8375352291 -2.079945644 0.4520385619
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 33
88.4693          103.0923          301.3967
373.4141         453.4717         615.9070
680.2008         899.4987         913.3253
947.3083         948.6890         965.0603
1032.1956        1034.9737        1084.8443

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1167.9590          1262.3906          1305.1039
1321.4261          1329.8601          1448.6147
1450.1292          1476.0799          1696.0347
1711.7911          3005.9649          3043.4491
3120.8611          3120.9299          3129.1043
3129.7765          3207.4104          3207.4763
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
Fragment      c5h7
RRHO
Geometry[angstrom]      12
C  -1.1010414736      0.3918722625      0.8234640968
C  -0.3631520631      -0.8239462751      1.462982238
C  1.0707741887      -0.6501660094      1.0310183231
C  -0.0133737739      1.136197524      0.0914150965
C  1.202988679      0.4885220714      0.2499527768
H  -1.583484021      1.0209968724      1.5815071743
H  -1.9013102667      0.0723672176      0.1447410417
H  -0.777380506      -1.7795464887      1.118858777
H  -0.4595285948      -0.8309072566      2.5556128554
H  1.8692946452      -1.3279976329      1.3019040122
H  -0.1777388973      2.0449229769      -0.4722088268
H  2.1372330834      0.8286777379      -0.1813115651
Core  RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]      30
123.2749          449.8385          597.4547
642.6361          726.9177          803.1772
810.9431          905.7597          912.4748
947.4334          992.0506          1027.4342
1072.4356          1105.1135          1141.8722
1221.8220          1273.6993          1300.2750
1317.5741          1400.1897          1469.6527
1478.1960          1492.7815          2996.2094
3007.3562          3009.1704          3029.4467
3179.0296          3201.0085          3212.7167
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  2
End
GroundEnergy[kcal/mol]  37.06
End
!-----c10h15_R5_ts1-----
Barrier      R5_ts1  R5  R5-1
RRHO
Geometry[angstrom]      25
C  -0.6880045154      0.5261849623      2.3700055788
C  -0.2308120251      -0.9646703523      2.2730742797
C  0.6659481889      -1.0180606683      1.0095986644

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C	-0.1994747092	-1.0851729995	-0.2691896096
C	-0.9777023701	0.2266652173	-0.4410511404
C	0.0653573564	1.1903075717	1.2429393858
C	1.3100201543	0.3841203946	1.0118053465
C	0.62054457	-1.2094221445	-1.5907664578
C	-0.6911082517	0.8067086535	-1.6519902907
C	0.4343502543	0.1198436569	-2.3735038312
H	-0.4145129022	0.9588531009	3.3427124593
H	-1.7732210017	0.6434746935	2.2816971831
H	-1.0729928162	-1.6584051905	2.2041910382
H	0.3465845135	-1.2480094292	3.1571855789
H	1.3801219985	-1.8456335795	1.0455888605
H	-0.8920597467	-1.9289755154	-0.1757493398
H	-1.9218552329	0.3968410749	0.0638481049
H	0.0194457806	2.2619097087	1.0816951964
H	1.836207536	0.634714032	0.0884030334
H	2.0287297817	0.4827729551	1.8402131318
H	0.2410821934	-2.0451387585	-2.183150494
H	1.6738670115	-1.4197754995	-1.3884255522
H	-1.1829361946	1.6922348488	-2.038173022
H	0.1953943649	-0.0563342531	-3.4288532062
H	1.3511010616	0.7274425199	-2.3758288977
Core RigidRotor			
SymmetryFactor 1.0			
End			
Tunneling Eckart			
ImaginaryFrequency[1/cm] 506.867			
WellDepth[kcal/mol] 23.18			
WellDepth[kcal/mol] 9.8			
End			
Frequencies[1/cm] 68			
89.8585	127.6297		
228.5033	242.6000	286.5056	
359.7249	433.0896	513.1179	
672.7395	679.0617	721.6800	
739.6307	753.0140	761.3680	
795.8593	826.6203	851.2044	
887.8938	899.7194	905.9340	
915.4493	935.9175	951.0360	
970.1868	974.6669	994.9392	
1026.0215	1043.9771	1056.9674	
1075.6663	1120.8395	1142.1797	
1156.2725	1169.0990	1201.5398	
1237.8405	1244.8045	1251.3195	
1276.7382	1290.8107	1297.8924	
1310.9744	1325.3393	1331.8664	
1341.5312	1363.1507	1377.0322	
1472.8539	1484.3206	1486.5957	
1496.7857	1506.7453	1510.5177	
2964.0575	2970.2482	2978.2889	
3016.4855	3019.2643	3029.9916	
3038.2142	3046.9838	3057.4208	

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3077.0330          3080.1186          3083.8742
3155.4848          3166.0707          3180.0728
ZeroEnergy[kcal/mol] 23.18
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R5-1_ts1-----
Barrier          R5-1_ts1  R5-1  R5-1_i1
RRHO
Geometry[angstrom] 25
C -0.4951672605 -1.5965212305 2.5947466062
C 0.7614057697 -1.2832794817 1.7141426602
C 0.5243460061 -0.0678108196 0.8437737217
C -0.3877546639 -0.1801871151 -0.3541769253
C -0.7361359219 1.1750814528 -0.9389006663
C -1.2762627469 -0.3182527805 2.740000711
C -0.5947352997 0.8566051484 2.5412494557
C 0.2714011318 -0.9032108907 -1.5824633052
C -0.1492832832 1.3960655486 -2.1130153077
C 0.6819771107 0.2199714908 -2.5681166389
H -0.1811580808 -2.0257894917 3.5538931527
H -1.1242609139 -2.3566411562 2.1199751376
H 1.0198297603 -2.1653010879 1.114274474
H 1.6229777664 -1.0938751102 2.3608089221
H 1.368138029 0.6062869513 0.7085627326
H -1.2917304187 -0.7201611694 -0.0480020494
H -1.3548651484 1.887055542 -0.4052016254
H -2.3583135098 -0.3457163108 2.6620841474
H -1.1347216169 1.7878120111 2.3934524878
H 0.4184105949 0.9867947566 2.9067741701
H -0.4741053188 -1.5485502898 -2.0552683155
H 1.1114705779 -1.5372730022 -1.2918535831
H -0.2217578038 2.3175039582 -2.6803971394
H 0.487975573 -0.0564502301 -3.6095589349
H 1.7525466674 0.4548703065 -2.507597888
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 562.6637
WellDepth[kcal/mol] 32.75
WellDepth[kcal/mol] 16.02
End
Frequencies[1/cm] 68
52.6042          77.8582
116.5444          126.1319          203.6295
267.9168          311.9982          380.1213
469.3338          506.3727          625.4033
637.9817          682.6022          701.4492
741.3107          784.9957          798.4459
815.0163          865.2019          896.0003

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902.9822          914.5947          923.7606
947.0063          964.6016          976.4894
980.0947          1008.0314         1036.2748
1045.5836         1094.3279         1115.0736
1130.9926         1162.1589         1196.5372
1204.0362         1227.7940         1256.4988
1264.8009         1279.9016         1310.8693
1322.2240         1334.6107         1336.2332
1373.5078         1396.9218         1419.0686
1478.3838         1484.3795         1494.6942
1502.0855         1553.1116         1678.9534
3002.6424         3003.2367         3008.7743
3012.2435         3035.5207         3037.2288
3050.2000         3059.4107         3088.2769
3111.5667         3119.6832         3153.2190
3166.2747         3184.7022         3193.0449
ZeroEnergy[kcal/mol] 46.13
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R5-1_ts7-----
Barrier          R5-1_ts7  R5-1_i1  R5-1_p4
RRHO
Geometry[angstrom] 25
C -1.0924312412 -0.7793581304 1.6563751915
C 0.6864599614 -1.3500866644 0.594768897
C 0.9381780723 -0.5532358087 -0.4993122536
C 0.3690952361 -0.7843991588 -1.8728586769
C -0.550361291 0.3535664223 -2.2951341759
C -0.8288626836 0.4251622922 2.3899150917
C -0.442989769 0.4831345774 3.6829518768
C 1.4462464022 -0.7682662597 -3.0093585128
C -0.0232620958 1.1112029863 -3.2547103997
C 1.333855666 0.6174942215 -3.6954199097
H -1.1802376191 -1.7003459676 2.2260650849
H -1.7449703495 -0.7208788764 0.79371221
H 0.3010298763 -2.3521925851 0.4264237638
H 1.2896153907 -1.2293815701 1.4869486014
H 1.4995148725 0.3692310061 -0.3639103592
H -0.1647984542 -1.7416753875 -1.8652195128
H -1.5010589934 0.5358021438 -1.8068596014
H -0.9119838458 1.3592271019 1.8373451092
H -0.2295994212 1.4269102968 4.1699138953
H -0.3449888064 -0.4148844621 4.2852448613
H 1.2085064773 -1.5544421091 -3.7302747856
H 2.4469845205 -0.9716094483 -2.6241043963
H -0.4861211963 2.0010794475 -3.6670985977
H 1.4225526461 0.5471698334 -4.7843294909
H 2.1219636452 1.3077090991 -3.3679839106
Core RigidRotor
SymmetryFactor 1.0

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End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  591.2671
WellDepth[kcal/mol]  21.75
WellDepth[kcal/mol]  12.9
End
Frequencies[1/cm]  68
26.7664          44.1166
61.7525          80.5402          125.7847
162.4207         251.3017         265.9860
374.2564         388.0697         423.4156
469.4963         642.2422         689.2185
691.9088         729.4253         765.5740
788.1214         799.3504         816.3388
873.1038         877.2735         913.5689
934.3361         955.0113         967.8524
980.3187         980.6951        1002.3278
1018.8950        1041.3844        1042.8946
1049.9388        1124.8326        1130.5120
1199.1756        1212.6307        1227.2739
1261.9829        1271.9547        1300.9074
1310.2091        1313.4955        1324.8460
1370.5659        1429.4770        1437.7145
1485.3744        1490.7934        1503.4246
1536.0852        1604.0966        1673.5479
3003.7758        3014.6204        3038.4614
3054.1375        3093.7649        3105.8438
3114.5745        3121.9141        3125.5771
3128.8634        3164.0210        3189.4423
3199.0394        3206.6171        3217.5136
ZeroEnergy[kcal/mol]  51.86
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----c10h15_R5-1_ts3-----
Barrier      R5-1_ts3  R5-1_i1  R5-1_i3
RRHO
Geometry[angstrom]  25
C  -0.9716694605   -1.0618717584   2.0612567765
C  -0.0361674722   -1.1885648419   0.8277259953
C  -0.2259284098   -0.123473108    -0.2106200114
C  -0.6082671494   -0.3691047082   -1.5022130381
C  -0.9993119636    0.7244267755   -2.4373206463
C  -0.778893363     0.2025742054   2.84993275
C  -0.3416645618    0.2603819462   4.1049293111
C  1.2135509833    -0.8031041285   -2.7994464279
C  -0.2056099013    1.1224443847   -3.4284824848
C  1.1320160931     0.4459688972   -3.6307386965
H  -0.8081354359   -1.9249650281   2.7150028806
H  -2.0093537822   -1.1161597656   1.7094358532
H  -0.1985129371   -2.1712565788   0.3723295628

```

```

H 1.0001367363 -1.1746712096 1.191804399
H 0.0366461032 0.8954345373 0.0650830866
H -1.0074563438 -1.3595175698 -1.7182453624
H -1.9610234145 1.2053713738 -2.2747722804
H -1.0194840252 1.1316075941 2.3364535247
H -0.2191732421 1.2050500507 4.6231210446
H -0.0935040017 -0.6378552852 4.6632714447
H 0.8581904583 -1.7280974252 -3.2408459084
H 2.0176055159 -0.9167033452 -2.0827781882
H -0.4925096956 1.9323883437 -4.0940417947
H 1.2610653254 0.2166042859 -4.6979947527
H 1.936809944 1.1475623581 -3.3772570372
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 443.3999
WellDepth[kcal/mol] 24.14
WellDepth[kcal/mol] 8.6
End
Frequencies[1/cm] 68
26.5304 46.9866
69.3378 84.4352 118.8582
165.3107 222.9934 290.1296
370.9904 382.6169 431.5622
472.6477 541.3678 545.5300
666.6296 703.5092 731.4679
790.1729 805.1649 820.1381
841.1235 869.4090 904.6351
944.9865 950.6284 973.1157
981.3732 989.3333 1028.2988
1041.4785 1057.6443 1090.1659
1094.5936 1126.7108 1183.0523
1194.5057 1246.5266 1257.9862
1284.0119 1309.7079 1318.2582
1324.1471 1338.4352 1363.2561
1385.3298 1454.5237 1460.2196
1480.7074 1483.2766 1486.5009
1554.0889 1702.6869 1706.3103
2983.9711 2990.6402 3007.7841
3016.2797 3047.4369 3053.1366
3099.5049 3119.7497 3125.8099
3127.2530 3128.9442 3135.5214
3155.6005 3205.2906 3219.4406
ZeroEnergy[kcal/mol] 54.25
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R5-1_ts4-----
Barrier R5-1_ts4 R5-1_i3 R5-1_p1
RRHO

```

```

Geometry[angstrom]    25
C   -1.3603876261    -0.2917309597    2.4718703862
C   -0.800338405    -0.9766338491    1.1965688237
C   -0.8306312477    -0.1163471059    -0.0336584146
C   -1.5774520092    -0.3649382421    -1.1164242961
C   -1.6281196165    0.4495496939    -2.3384084723
C   -0.5951886028    0.9281779339    2.902629916
C    0.1047101395    1.0306125032    4.0291041227
C    2.2347554537    0.6312626784    -3.6817580046
C   -0.6547021687    1.1483262145    -2.8965344443
C    1.6364455898    0.7434771924    -2.4765677748
H   -1.3637007895    -1.0232647486    3.2862869456
H   -2.4052159082    -0.0177270217    2.2808924445
H   -1.3709488455    -1.8930289704    1.0144541412
H    0.2336594011    -1.280674403    1.402949438
H   -0.2133659685    0.7787799693    -0.024760687
H   -2.2388498621    -1.2304301705    -1.1035321595
H   -2.5999636095    0.4568538997    -2.8467584063
H   -0.6275374926    1.7814301364    2.2277217705
H    0.6413208052    1.9370572643    4.286444725
H    0.1632113446    0.2110365789    4.7397467511
H    2.6591272177    1.4906047904    -4.189407969
H    2.2686773261    -0.3144386345    -4.2110471035
H   -0.6449390469    1.7525889013    -3.7928130153
H    1.6892920917    1.6684407528    -1.9141197893
H    1.3100878291    -0.1318774039    -1.928607928
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm]  310.0255
WellDepth[kcal/mol]  36.57
WellDepth[kcal/mol]  2.63
End
Frequencies[1/cm]  68
23.3287            46.3460
50.3672            77.3114            89.1112
110.4116           135.3656            194.6160
226.1179           261.2250            294.2821
343.5486           382.5916            417.9746
469.3939           609.7129            664.5321
684.7795           799.1716            829.4266
847.9044           858.6403            881.6176
885.0751           907.6507            942.7716
946.8481           982.4978            996.1718
1006.2110          1021.5247           1035.2649
1053.6319          1104.4496           1132.2176
1202.7906          1236.2028           1257.0763
1267.0402          1315.0999           1320.8946
1325.3735          1339.0577           1346.2418
1375.4681          1454.4252           1467.9654
1483.2597          1486.4177           1592.0302

```

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1637.7776          1699.1483          1706.3034
3004.5372          3011.1716          3014.0104
3054.7775          3057.8355          3115.0914
3120.2195          3128.0033          3129.2508
3138.9885          3143.3096          3205.1773
3206.2255          3216.6116          3233.3777
ZeroEnergy[kcal/mol] 82.22
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R5-1_ts2-----
Barrier          R5-1_ts2  R5-1  R5-1_i2
RRHO
Geometry[angstrom] 25
C -0.7275598116    -1.4803408799    3.0935819798
C 0.6194977082     -1.5363985474    1.2810893582
C 0.3296997947     -0.1245931541    0.8089231476
C -0.5425394142    -0.1224439511    -0.4769871587
C -0.8547118895    1.2716932758     -0.9873336331
C -1.302194764     -0.3326736419    2.6107242762
C -0.3496735904    0.6504099488     2.0021891096
C 0.17424928       -0.7630836807    -1.7053582059
C -0.2053396355    1.5650588765     -2.112283829
C 0.6463949893     0.4162166212     -2.5942868974
H 0.2130410552     -1.4369085131    3.6321332144
H -1.3213951552    -2.3690635333    3.2853764659
H 0.2221031125     -2.3717267168    0.7154636596
H 1.572278619      -1.7325700192    1.7625263608
H 1.2719499745     0.3847719422     0.5691778039
H -1.4646872467     -0.6696267346    -0.2459262416
H -1.5148462801     1.9554606708     -0.4666117663
H -2.3448071152     -0.3250889353    2.307241551
H -0.8169723354     1.5788344451     1.671355662
H 0.4311464845     0.9208529826     2.7227465906
H -0.5411846153     -1.3714848459    -2.264603593
H 0.9942391267     -1.4203168637    -1.409319836
H -0.2524128195     2.5193009706     -2.6256239367
H 0.509525522       0.2093539327     -3.6605568588
H 1.7128810059      0.639051351      -2.4601662232
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 568.9239
WellDepth[kcal/mol] 34.42
WellDepth[kcal/mol] 15.77
End
Frequencies[1/cm] 68
51.3669            63.8744
99.7139            187.2113            263.4830
286.6127           343.4718            399.6651

```

460.3183	492.6640	552.5029
598.1314	675.8102	698.1791
737.1189	777.4460	791.7454
805.5464	864.6010	873.0135
894.3394	917.7889	922.0051
932.0538	945.8651	965.1790
979.1563	987.9522	1002.1133
1046.8159	1049.6449	1098.1807
1124.9244	1136.0580	1183.8840
1200.5012	1222.7915	1239.0532
1265.4567	1287.7370	1290.3972
1316.5631	1323.8310	1328.9878
1370.1075	1382.2386	1418.3228
1465.3876	1485.9361	1499.1406
1503.8117	1551.4621	1678.9562
2995.8066	3002.7474	3012.1130
3020.8061	3038.2635	3053.1073
3089.5431	3096.2169	3116.0764
3120.4623	3149.4572	3165.9185
3191.8662	3193.0375	3209.2400

ZeroEnergy[kcal/mol] 47.80

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c10h15_R5-1_ts8-----

Barrier R5-1_ts8 R5-1_i2 R5-1_p4

RRHO

Geometry[angstrom] 25

C	-1.400626311	-0.9151715641	3.6220542261
C	1.6620643582	-1.2795464623	1.4520382389
C	1.1069044965	-0.1395954335	0.9067070677
C	0.0589800982	-0.2473269058	-0.201669417
C	-0.5617284651	1.0826458612	-0.5867243844
C	-1.2059439296	0.1057194247	2.7593279637
C	0.0440024787	0.7755271898	2.5413793968
C	0.6710811599	-0.7169876036	-1.5645470454
C	-0.1445593182	1.5197415201	-1.7734152096
C	0.8121896113	0.5565926834	-2.4338395454
H	-2.3654106692	-1.3979332115	3.7215804234
H	-0.5981781365	-1.2819120303	4.2540118671
H	1.1525724404	-2.2358068044	1.3985272668
H	2.5620498948	-1.2347566664	2.0543216902
H	1.7484355279	0.7373545299	0.8434336563
H	-0.6992781966	-0.9624078019	0.135168956
H	-1.2426175018	1.6224939686	0.0604109648
H	-2.0485358377	0.4247496183	2.1488589829
H	0.019450342	1.764785107	2.0980202158
H	0.8183822208	0.6429594733	3.2882658378
H	-0.0319359851	-1.4030802116	-2.0445573961
H	1.6118486998	-1.2509724431	-1.4277410942
H	-0.4309829935	2.4651279214	-2.2211158148

```

H 0.5642447191 0.3705170216 -3.4835996676
H 1.8344842967 0.956437819 -2.42521218
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 578.6086
WellDepth[kcal/mol] 20.79
WellDepth[kcal/mol] 13.86
End
Frequencies[1/cm] 68
51.8833 64.3355
93.6393 106.6713 154.1540
228.7927 252.2958 288.6897
385.8168 396.9985 432.7407
482.0093 510.7394 642.6935
682.3462 729.9419 745.9281
782.7128 792.6010 806.0952
856.1307 878.5306 885.0819
916.4305 945.5953 960.4516
980.2646 986.1877 1001.7983
1017.9121 1034.6267 1055.7304
1070.0544 1114.1811 1138.5376
1192.3334 1213.5222 1222.9194
1256.1179 1278.7037 1302.0809
1314.2377 1316.2957 1328.5033
1380.5502 1420.8518 1436.3047
1486.5329 1497.0901 1503.7326
1520.6684 1603.4352 1678.9621
3003.9363 3025.4706 3040.3327
3055.7277 3103.3074 3113.1821
3122.8720 3127.2444 3128.7560
3133.5027 3168.2943 3195.3443
3211.6202 3217.4722 3219.7266
ZeroEnergy[kcal/mol] 52.82
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R5-1_ts9-----
Barrier R5-1_ts9 R5-1_i2 R5-1_p5
RRHO
Geometry[angstrom] 25
C -1.3066170476 -1.1463272388 2.7024559444
C 1.6541029509 -1.3203762774 1.2310441559
C 1.0312946628 -0.1378169234 0.868005998
C -0.3808466904 -0.5670468125 -0.674584074
C -1.0393646677 0.6823605886 -0.987524125
C -0.8125949151 0.0885822732 2.7289349594
C 0.2658876948 0.7072211143 1.8756106667
C 0.4522316169 -0.9268483797 -1.8969340965
C -0.5123896301 1.261565357 -2.0912179614

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C 0.5734572328 0.4021651166 -2.692610548
H -2.1000823335 -1.4383408862 3.3814596629
H -0.947212221 -1.908033489 2.0221514611
H 2.4127609467 -1.7659398871 0.5984187027
H 1.3545162889 -1.8830713872 2.1059223188
H 1.5690746322 0.473798664 0.1468376585
H -0.918713953 -1.3469169299 -0.1530540154
H -1.8344565591 1.1066222937 -0.3863404539
H -1.2318973368 0.7838152521 3.4556303736
H -0.1768349061 1.5630519123 1.3513349246
H 1.002177926 1.1579134555 2.557402387
H -0.0890217831 -1.6692450515 -2.4959587343
H 1.4192384739 -1.3703514098 -1.6485987796
H -0.8075601487 2.2207455832 -2.4991947134
H 0.4463426467 0.2579676024 -3.7705841393
H 1.5598341196 0.8673484597 -2.5635555726
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 598.817
WellDepth[kcal/mol] 21.03
WellDepth[kcal/mol] 21.03
End
Frequencies[1/cm] 68
24.9325 82.5710
101.3694 142.5142 179.9565
199.6542 237.5393 277.9334
303.5758 376.8547 468.8418
511.3979 571.1861 650.8598
692.9963 728.8467 763.8527
797.8394 803.6395 829.9639
871.5191 905.2655 926.1835
937.0190 946.1413 954.7238
963.4002 992.5559 1016.4206
1047.2172 1050.8174 1063.8475
1083.8163 1101.2527 1122.0828
1156.4365 1222.5672 1238.5965
1268.9397 1282.2013 1304.7293
1325.0838 1333.2721 1382.4834
1391.3921 1413.2220 1455.0074
1471.9479 1476.1323 1495.1451
1522.3635 1564.1316 1708.7189
2982.3907 2995.9220 3009.3572
3019.4716 3040.2283 3070.8892
3108.2748 3110.1007 3139.8793
3143.2892 3176.5416 3191.9697
3202.9063 3220.9394 3230.2678
ZeroEnergy[kcal/mol] 53.06
ElectronicLevels[1/cm] 1
0 2
End

```

!-----
End

R5_secondary_p4-3

```
!-----r5-1-p4_r3-----
Well          r3
Species
RRHO
Geometry[angstrom]  16
C  0.7201747136  -1.3731636071  2.0839578995
C  0.0618519595  -0.3269784603  1.5115545
C  0.1553743199  0.0703443035  0.1587455061
C  -0.5300672134  1.1598562213  -0.4378419835
C  1.0077333634  -0.5983042786  -0.9018834526
C  -0.2288024582  1.2851129431  -1.7625732021
C  0.7472077895  0.2226506042  -2.1973941414
H  1.3940278928  -2.005125998  1.5169250673
H  0.5916401977  -1.6105868806  3.1324486824
H  -0.5997798136  0.2661720887  2.1401484727
H  -1.2089344167  1.8069099198  0.1061238315
H  0.730886066  -1.6510453591  -1.024780103
H  2.0664414328  -0.589530617  -0.6206856954
H  -0.6265995057  2.0394607579  -2.4294082559
H  0.3346681761  -0.3980955898  -3.0015360085
H  1.668437752  0.6619892795  -2.5979882665
Core RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  42
98.1654          163.9919          209.7451
293.2540          463.9855          478.4019
606.4493          624.7706          708.2213
777.3120          818.7660          837.1156
852.7861          918.4559          944.0304
977.0786          987.3321        1007.4033
1033.8823         1093.0705         1155.2103
1225.2871         1231.5914         1265.2093
1278.6450         1311.7855         1342.1975
1412.9012         1438.1182         1470.2402
1487.0137         1505.8794         1578.2663
3006.9272         3021.8126         3021.8257
3047.3392         3123.3549         3142.3662
3176.5546         3202.5950         3228.9770
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----5-7-c_i1-----
Well          i1
Species
RRHO
```

```

Geometry[angstrom] 16
C 0.5672277255 -1.189960237 2.4452897224
C 0.382914143 -0.1701109522 1.6064907978
C 0.4372330969 -0.2320270203 0.1224367275
C -0.3828877999 0.7224438724 -0.5602279132
C 1.2089178483 -1.1754385363 -0.4996018568
C -0.3956292281 1.109939237 -1.9270252624
C 0.5330838507 0.8900586515 -2.8977021001
H 0.760129012 -2.1979348729 2.0939452477
H 0.5189176691 -1.0477659584 3.51850519
H 0.1500277453 0.8073085262 2.0231559345
H -1.1121506943 1.2313019426 0.0642853424
H 1.1728680662 -1.3291641463 -1.5681560204
H 1.8521701423 -1.8312089863 0.0730707544
H -1.2573466139 1.7108984553 -2.2119379052
H 0.3759101381 1.2715901833 -3.8992476236
H 1.47287516 0.3897351734 -2.707468183
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 42
65.1751 98.6664 183.2178
236.0308 309.6673 352.8148
431.5984 512.7836 570.9181
619.8329 652.0096 725.9499
810.6401 855.2230 865.3054
880.4450 947.7372 950.2458
994.6053 1027.5396 1028.6610
1082.1456 1158.8742 1238.1707
1284.0943 1331.9530 1369.3585
1439.1336 1456.6425 1464.9066
1555.7638 1580.5961 1686.4746
3116.8964 3128.1743 3138.0520
3144.5810 3151.6428 3162.2229
3218.6491 3238.5920 3255.5245
ZeroEnergy[kcal/mol] 23.46
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----5-3-h_i2-----
Well i2
Species
RRHO
Geometry[angstrom] 16
C 0.1579264789 -1.5826737286 1.6703994803
C 0.2876101307 -0.2673082873 1.5331982743
C 0.79382339 0.462717116 0.3007240883
C -0.2898041389 1.2945532083 -0.375755994
C 1.2843936243 -0.3842485851 -0.8391643481
C -0.4154522991 1.005070416 -1.6689967045

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C 0.5591739843 -0.0644531982 -2.1108984114
H 0.4184113034 -2.2681807064 0.8711581174
H -0.2179344406 -2.0176436859 2.5897013815
H 0.0110686893 0.3817480974 2.3629708641
H -0.8795229315 2.0250625165 0.1656183993
H 2.1093637749 -1.0799603378 -0.7628510855
H 1.5966268899 1.1369521956 0.6553443301
H -1.1251664338 1.4675015153 -2.3450489956
H 0.045560012 -0.9370600107 -2.5463089585
H 1.2337009663 0.295923475 -2.9049774379
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 42
85.2125 121.1109 235.6689
302.1915 372.1194 431.4886
559.6754 620.5205 686.7593
764.2646 806.9783 874.0126
926.5353 928.6234 946.1714
959.9680 969.5296 1001.9923
1034.5795 1036.0015 1088.4924
1128.6473 1133.8340 1242.5462
1279.1778 1295.7756 1310.3665
1332.9434 1385.2087 1439.6418
1459.3739 1673.3389 1701.1977
2891.6937 2947.3276 2949.8606
3113.9949 3133.6594 3171.7392
3196.1000 3202.6592 3213.0037
ZeroEnergy[kcal/mol] 24.31
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c2h3_c5h6_R5-1-p4_p1-----
Bimolecular R5-1-p4_p1
Fragment c5h6
RRHO
Geometry[angstrom] 11
C 0.0103684493 -1.0048217008 -0.9087252484
C -0.7782563238 0.0286243202 -1.0827853865
C 0.7955820167 -2.0280598777 -0.7379460132
C -0.4256956778 1.2902651927 -1.7551810891
C 0.7524161938 1.5995336989 -2.3017230874
H -1.792595263 -0.0455725539 -0.695830965
H 0.8547170648 -2.8275728417 -1.4719317093
H 1.4205343804 -2.1232958816 0.1462585317
H -1.2281358977 2.0219481653 -1.7930620316
H 0.9125097547 2.5601100307 -2.7757840678
H 1.5872751467 0.9067309605 -2.2921008868
Core RigidRotor
SymmetryFactor 1

```

```

End
Frequencies[1/cm]  27
62.3720           151.4550           321.2499
395.1117           503.4859           654.9408
715.6216           875.7172           910.0005
912.8139           936.2929          1010.0893
1028.0011          1049.5005          1154.8452
1337.7637          1374.5285          1444.7811
1474.7261          1679.2021          2030.6036
3103.7278          3122.0783          3135.9242
3149.6656          3172.7199          3223.9301
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment          c2h3
RRHO
Geometry[angstrom]  5
C  -2.6815309499   -1.8887734891   -1.1309235268
C  -1.725733176    -1.3518528792   -0.4241833636
H  -3.0692157655   -1.4200651964   -2.0332260024
H  -3.1437000229   -2.8401606701   -0.8523521394
H  -1.1628990858   -1.5707617651    0.4715150322
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  9
712.2118           819.4319           921.7170
1046.2369           1391.3607          1651.0507
3037.2336           3133.0072          3234.0563
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol]  86.1
End
!-----c2h3_c5h6_R5-1-p4_p2-----
Bimolecular  R5-1-p4_p2
Fragment      c5h6
RRHO
Geometry[angstrom]  11
C  1.7739473074    -0.6818466093    -0.7221071247
C  0.7200203695    -1.0943582551    -1.4506225047
C  -0.2941048379    -0.0324120696    -1.4821037331
C  0.1452095209     1.0236956202    -0.7726629161
C  1.5088975741     0.7111879701    -0.2184053795
H  2.6777413601    -1.2383555006    -0.515109658
H  0.6186967493    -2.0533819236    -1.9425843223
H  -1.2418186269    -0.1051309279    -2.0003409082
H  -0.3745603273     1.9578940938    -0.609861296
H  2.2675009981     1.4252972695    -0.5668910274
H  1.5278529127     0.7618083327     0.87884187

```

```

Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 27
348.5708          524.1051          681.3317
711.8753          817.0247          818.8020
917.6681          924.4172          953.9591
955.9506          970.7216        1012.6714
1112.1153         1124.7078          1130.0719
1265.2943         1314.9663          1397.2719
1414.9257         1551.9926          1639.1108
3009.5972         3031.2355          3186.6692
3196.7126         3215.2104          3221.8506
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment          c2h3
RRHO
Geometry[angstrom] 5
C -2.6815309499   -1.8887734891   -1.1309235268
C -1.725733176    -1.3518528792   -0.4241833636
H -3.0692157655   -1.4200651964   -2.0332260024
H -3.1437000229   -2.8401606701   -0.8523521394
H -1.1628990858   -1.5707617651    0.4715150322
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 9
712.2118          819.4319          921.7170
1046.2369         1391.3607          1651.0507
3037.2336         3133.0072          3234.0563
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 55.44
End
!-----h_c7h8_R5-1-p4_p2-3-----
Bimolecular      R5-1-p4_p2-3
Fragment          c7h8
RRHO
Geometry[angstrom] 15
C 0.1739997967    -1.5460752179    1.8122391887
C 0.324680931     -0.2480558607    1.5692075473
C 0.7291372666     0.3778604652     0.2539784716
C -0.3525376285    1.2521540983     -0.3524921934
C 1.0763409906     -0.5486182889     -0.8838026578
C -0.5545218328     0.8878320403     -1.6301207446
C 0.3404145728     -0.2287387356     -1.9629285648
H 0.340256082      -2.2980345338     1.0494251559
H -0.1316815966    -1.898276535      2.7910915924

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```

H  0.1383893488    0.4639423486    2.3711994425
H -0.8602527592    2.0365119332    0.1921908762
H  1.8316078388   -1.3197171321   -0.8190626929
H  1.6052243881    1.0217019264    0.4488942797
H -1.259254816    1.3360987368   -2.3189316592
H  0.391994327   -0.7034179717   -2.9346653763
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  39
96.6006           162.7769           240.7472
410.1090          530.2283           597.9005
633.7299          702.8545           729.6778
815.8618          843.7614           888.5808
947.4147          953.6961           962.1693
987.9126         1008.7303          1020.2519
1037.3837         1088.8241          1111.2667
1130.4259         1209.6479          1273.9107
1311.0856         1334.3748          1400.3645
1446.8763         1557.3187          1641.3649
1703.5818         2949.9858          3121.5826
3139.7621         3187.0508          3197.1772
3215.6293         3219.3046          3222.2819
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment          H
Atom
Mass[amu]  1
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol]  54.51
End
!-----h_c7h8_R5-1-p4_p3-----
Bimolecular  R5-1-p4_p3
Fragment      c7h8
RRHO
Geometry[angstrom]  15
C  0.7443928714   -1.3490457846    2.1192390514
C  0.0996445535   -0.3097045997    1.5721375373
C  0.114366723    0.0698714649    0.1744554777
C -0.5402063272    1.1245058925   -0.379086726
C  0.8655128784   -0.6433625597   -0.9280943541
C -0.2794791736    1.177991565   -1.8144253549
C  0.5348998466    0.16078149   -2.1568642189
H  1.3585019576   -2.0213424081    1.5296606747
H  0.6755628424   -1.5580941948    3.17972883
H -0.5007707266    0.3276416175    2.218356614
H -1.1651757639    1.8260902994    0.1600768602
H  0.5471698061   -1.6886300362   -1.0280933515

```

```

H 1.9455396573 -0.6674188552 -0.7360273234
H -0.6852244528 1.9251838977 -2.4843441976
H 0.9079624739 -0.0671847843 -3.1459492301
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 39
124.3028 211.0619 238.3125
366.5748 479.7569 525.8222
618.2448 663.2373 704.7735
826.0168 884.6607 893.9810
910.5914 927.3268 957.2569
958.3030 1013.9583 1026.6553
1035.5369 1123.7193 1134.4806
1214.4226 1255.3239 1321.0912
1340.4518 1393.5409 1419.8632
1447.2796 1553.6099 1628.4275
1679.9293 3021.7172 3047.3312
3126.7072 3139.2148 3187.8486
3199.4255 3220.6212 3221.6809
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 46.66
End
!-----h_c7h8_R5-1-p4_p4-----
Bimolecular R5-1-p4_p4
Fragment c7h8
RRHO
Geometry[angstrom] 15
C 0.761986697 -1.3064834751 2.1074761465
C -0.0498652816 -0.4674278355 1.4597467341
C 0.0941356575 -0.0284563114 0.0688934584
C -0.4511705723 1.24700915 -0.438979479
C 0.6978615679 -0.6683228495 -0.9616250155
C -0.165535167 1.3788116685 -1.7451002219
C 0.59774856 0.1671289852 -2.2050692767
H 1.6451048532 -1.725525301 1.6368189161
H 0.5713767701 -1.5929813261 3.134970323
H -0.8965848625 -0.0458462594 1.9983572911
H -0.9875174569 1.9601105742 0.1753857783
H 1.1577934248 -1.6464698617 -0.9278449095
H -0.4236412766 2.2113932066 -2.3851636441
H 0.0809339371 -0.3622095875 -3.0175195143
H 1.5870493433 0.4340976336 -2.603045741

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```

Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 39
79.0512 196.5603 233.1919
358.3962 443.4521 547.5681
639.5354 681.1070 718.0940
790.7956 823.0251 913.0510
924.0304 936.9707 940.4218
950.4558 989.9255 1027.3031
1074.6409 1101.5670 1123.8526
1190.7566 1260.3316 1281.6421
1332.2331 1377.2871 1414.5857
1457.5133 1569.9916 1650.5216
1688.7259 3004.5623 3024.3769
3123.9892 3136.4603 3186.4708
3210.5755 3217.0142 3219.5863
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 49.54
End
!-----5-7-c_ts1-----
Barrier ts1 r3 i1
RRHO
Geometry[angstrom] 16
C 0.356933506 -1.5494152543 2.0811749128
C -0.1286553654 -0.5296713064 1.347019824
C 0.5228294321 0.1038142889 0.2188965448
C -0.0168525423 1.3424284295 -0.358732492
C 1.5055516893 -0.4847180942 -0.5593974356
C -0.0808227689 1.3649624308 -1.7055574032
C 0.3286748884 0.1794961383 -2.4683986713
H 1.3360796064 -1.976733079 1.8948969883
H -0.2170102601 -1.9755849529 2.8948492067
H -1.0935712768 -0.1127845834 1.6287958655
H -0.4002018217 2.1485735673 0.2582063267
H 1.7652153193 -1.5315760429 -0.428957864
H 2.2369111998 0.1206475667 -1.0756200019
H -0.4326233154 2.2525731018 -2.228940516
H -0.3189534113 -0.6921451072 -2.4519006353
H 0.9207553913 0.2997982365 -3.3705217944
Core RigidRotor
SymmetryFactor 1.0
End

```

```

Tunneling      Eckart
ImaginaryFrequency[1/cm]  681.9965
WellDepth[kcal/mol]  49.7
WellDepth[kcal/mol]  26.24
End
Frequencies[1/cm]  41
97.7879          161.0184
223.3190          304.1245          400.3268
452.1398          493.0909          529.6453
651.5678          669.2342          691.8030
774.3214          798.0711          880.4592
893.3107          921.2863          960.8820
985.9950          1006.5278          1009.2082
1060.9790          1084.9872          1170.7517
1231.2136          1318.9657          1372.0174
1388.4525          1449.6922          1451.9067
1521.0431          1596.9105          1629.7318
3108.4493          3116.9490          3123.8040
3131.1082          3138.9388          3169.0871
3194.8506          3223.0204          3226.3539
ZeroEnergy[kcal/mol]  49.7
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----2-3-c_ts1-1-----
Barrier      ts1-1  i1  R5-1-p4_p1
RRHO
Geometry[angstrom]  16
C  0.7531112521  -0.6437233395  2.5601614641
C  0.8583639626  0.057261979  1.4604330477
C  0.0802028352  -0.9221765107  -0.7227051744
C  -0.7722708628  0.0480881703  -1.0450829947
C  0.8010630459  -2.0110147565  -0.7383539195
C  -0.4453110189  1.2515960018  -1.8020320832
C  0.7629954988  1.5977796426  -2.2686711886
H  0.4064978391  -1.6753897676  2.5600934419
H  1.0117863282  -0.2293064524  3.5384195053
H  1.145781035  1.0729333999  1.2255173464
H  -1.7815889653  -0.0210529372  -0.6456450302
H  0.6950867733  -2.7141204267  -1.5621878673
H  1.5133870737  -2.2571901645  0.0390007182
H  -1.2851362739  1.9158193163  -1.9882267643
H  0.9023693112  2.51136631  -2.8332788109
H  1.6379224268  0.9787948671  -2.1016288385
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  335.4791
WellDepth[kcal/mol]  63.24
WellDepth[kcal/mol]  0.6

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```

End
Frequencies[1/cm]  41
30.7716           47.6085
110.8524          140.8139          153.9497
164.5404          252.3400          297.7411
401.3569          520.4714          654.3732
707.7377          755.9896          862.5331
872.6662          894.3591          920.9444
923.1709          927.0995          996.6468
1020.4376         1038.3372         1061.4373
1141.8480         1328.7917         1371.5883
1390.5259         1442.6218         1459.8310
1639.9388         1646.2040         1942.2522
3040.0193         3105.9803         3125.7493
3130.5140         3136.5737         3147.6639
3201.9124         3217.5782         3225.9737
ZeroEnergy[kcal/mol]  86.7
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----5-3-h_ts2-----
Barrier      ts2  r3  i2
RRHO
Geometry[angstrom]  16
C  0.451689035  -1.5423635808  2.014389248
C  0.103113239  -0.3292220674  1.5514667416
C  0.3342820443  0.1775184603  0.2081602166
C  -0.4583679868  1.2470484787  -0.4233193976
C  1.0081282954  -0.5291843593  -0.9223334244
C  -0.3279112965  1.2292033908  -1.7596170352
C  0.5916159147  0.1162848548  -2.219454387
H  0.9179235919  -2.2891347049  1.3814785247
H  0.2693317614  -1.8208446392  3.044882746
H  -0.3768563496  0.3734292667  2.2287184095
H  -1.053366196  1.9483110445  0.1478838324
H  1.5526037148  -1.4542776432  -0.8139124597
H  1.5166780851  0.4459168683  -0.0131043366
H  -0.7893910105  1.9286536361  -2.4449668753
H  0.0696367384  -0.5979561367  -2.8812221556
H  1.4369404193  0.4902731312  -2.8185586474
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1797.4484
WellDepth[kcal/mol]  54.34
WellDepth[kcal/mol]  30.03
End
Frequencies[1/cm]  41
119.5853          198.5280
224.8985          321.2948          457.9352

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517.2806          543.6047          615.2043
678.9193          750.5533          790.1121
864.8307          875.2950          919.3761
933.9329          942.5181          979.7595
985.5742        1036.4194        1105.7657
1128.7725        1152.1756        1211.7597
1237.4330        1302.5465        1307.5829
1340.8341        1398.7732        1456.6874
1463.6987        1601.3799        1639.4904
2184.5607        2902.9662        2946.1578
3131.2280        3140.5579        3186.7240
3208.2832        3222.3788        3236.3559
ZeroEnergy[kcal/mol]  54.34
ElectronicLevels[1/cm] 1
0  2
End
!-----
!-----2-3-c_ts2-1-----
Barrier      ts2-1  i2  R5-1-p4_p2
RRHO
Geometry[angstrom]  16
C  0.1666328286  -1.7450863036  1.7804005602
C  -0.0143256037  -0.4508431659  1.6780603169
C  1.093566057   0.7397136162  0.0132857924
C  -0.051750296  1.527151425  -0.4879872318
C  1.4373857448  -0.1715351122  -0.9523854449
C  -0.438723394  1.0520889139  -1.6819469997
C  0.4525698407  -0.0946490241  -2.0848618442
H  0.8178739763  -2.2898795865  1.1006333975
H  -0.3286957142  -2.3397686159  2.5507235028
H  -0.6206460237  0.2430310661  2.2483204361
H  -0.5112313835  2.3432852429  0.0549061279
H  2.273010424   -0.8566839449  -0.9186219926
H  1.7307828738  1.048592135  0.8302632126
H  -1.2690485649  1.4066726236  -2.2777373588
H  -0.1167756667  -1.0278343796  -2.2091320034
H  0.9491539016  0.0837451102  -3.0488074712
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  361.8236
WellDepth[kcal/mol]  34.59
WellDepth[kcal/mol]  3.46
End
Frequencies[1/cm]  41
36.0722          101.3281
127.4551          208.6729          316.2788
360.8548          518.0527          660.7460
705.2409          786.2534          807.9533
814.1085          881.6502          890.5739
918.7923          923.6480          936.4830

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953.1276          967.6740          1002.4464
1085.2804         1102.2401         1122.9494
1128.5637         1272.1636         1310.2511
1388.8058         1390.5686         1419.9767
1473.7874         1617.8905         1645.2521
2991.6200         3013.1268         3056.9666
3141.0214         3186.7912         3188.5026
3199.1977         3213.3384         3220.3698
ZeroEnergy[kcal/mol] 58.9
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----3-13-h_ts2-2-----
Barrier          ts2-2  i2  R5-1-p4_p4
RRHO
Geometry[angstrom] 16
C 0.3437404448 -1.6154859838 1.9606555516
C 0.2261936594 -0.3586565519 1.5312456193
C 0.3437154735 0.0776904905 0.1280014988
C -0.4957654417 1.1531128762 -0.4585396505
C 0.9597500562 -0.5764222983 -0.9103452947
C -0.3527530644 1.1679378702 -1.7911041789
C 0.6122688606 0.0900124193 -2.2068848129
H 0.5342259113 -2.4384395249 1.2803757187
H 0.2462666907 -1.8598548037 3.0118409232
H 7.796305E-4 0.4252614505 2.2495919718
H -1.114384827 1.8168459661 0.1318992845
H 1.6440040541 -1.4082751883 -0.8182788453
H 1.7815942023 1.2501812401 0.6016763272
H -0.8321927051 1.847005646 -2.483065944
H 0.1714654314 -0.6117060142 -2.9286976832
H 1.5008706235 0.5087924064 -2.7032574859
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 764.1276
WellDepth[kcal/mol] 31.2
WellDepth[kcal/mol] 5.97
End
Frequencies[1/cm] 41
95.6618          193.5674
236.6176         338.9726         394.8082
425.7064         475.7983         569.9166
630.4885         681.9117         706.2015
774.9761         813.8917         908.3505
920.8787         938.4741         941.9782
953.1204         988.0951        1027.6489
1067.4424        1103.4966        1125.4343
1182.6026        1257.0040        1287.3018
1330.2346        1367.2479        1416.7249

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1451.5090          1527.9717          1627.4583
1688.6144          2990.3972          3013.7627
3134.1649          3143.1778          3192.6403
3214.1137          3217.8063          3220.7326
ZeroEnergy[kcal/mol] 55.51
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----7-16-h_ts2-3-----
Barrier          ts2-3  i2  R5-1-p4_p2-3
RRHO
Geometry[angstrom] 16
C 0.1802650539 -1.5485706249 1.8168220865
C 0.3262270891 -0.2503791104 1.5725503046
C 0.7237201406 0.3767319087 0.2552834645
C -0.3612885674 1.2450876481 -0.3549226059
C 1.0747686984 -0.5489510496 -0.878045383
C -0.5466817629 0.9023435859 -1.6386738562
C 0.372133858 -0.1959134881 -1.9862768024
H 0.3454333731 -2.3014765606 1.0545895854
H -0.1193673602 -1.9010584321 2.7973151421
H 0.1409753024 0.4622192969 2.3740370356
H -0.8781527193 2.0215710225 0.1925579057
H 1.818898228 -1.33001852 -0.8100380909
H 1.5978038921 1.025894734 0.4484740196
H -1.2410020627 1.3590864573 -2.3315631477
H 0.3600637463 -0.7313995944 -2.9258869925
H 1.7759820907 0.8828327268 -2.9911096656
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 548.4871
WellDepth[kcal/mol] 34.04
WellDepth[kcal/mol] 3.84
End
Frequencies[1/cm] 41
87.3134          149.6284
227.7415          286.4515          302.0546
424.1844          540.3407          594.4278
630.2787          714.2850          729.6123
814.3560          844.3183          888.0020
947.6949          954.5738          968.7130
982.9275          1007.8997          1018.3816
1036.3676          1088.9438          1106.8124
1125.4908          1211.4341          1273.2789
1308.9281          1334.9153          1396.1453
1447.2851          1518.7735          1621.4960
1703.6837          2934.2800          3122.8881
3139.2398          3193.5428          3202.8078
3217.0883          3219.0643          3225.0203

```

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ZeroEnergy[kcal/mol]  58.35
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----7-16-h_ts3-----
Barrier      ts3   r3   R5-1-p4_p3
RRHO
Geometry[angstrom]  16
C  0.7905255051  -1.3138624439   2.0777502218
C  0.1355959156  -0.2716427966   1.5590755083
C  0.0915481346   0.0618134293   0.1462942742
C  -0.5709737345   1.1035401118   -0.4131834581
C  0.772353227   -0.7184792583   -0.9468269864
C  -0.3634902936   1.103940103   -1.8527490273
C  0.4605026887   0.0807529132   -2.1838317623
H  1.3526289471   -1.9999563877   1.4530427191
H  0.7834778929   -1.5096618107   3.1423395426
H  -0.4155685599   0.393633619   2.2188220014
H  -1.1638164438   1.8301819168   0.1278660528
H  0.3452336034   -1.7260647495   -1.0250402426
H  1.8456672995   -0.8357211544   -0.7725141994
H  -0.7858320603   1.825828342   -2.5384148213
H  0.7433269101   -0.2181873519   -3.1832445765
H  2.2630829681   1.1535515181   -2.1335712462
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  531.0447
WellDepth[kcal/mol]  49.85
WellDepth[kcal/mol]  3.19
End
Frequencies[1/cm]  41
117.5661          179.8188
212.4746          263.2847          344.0056
408.4654          478.3596          526.3284
622.3672          669.8249          759.9890
825.9851          891.8229          909.9486
920.1517          951.6550          965.2888
969.8385          1019.6680         1032.0546
1041.3460          1119.0039         1140.2099
1222.5050          1254.4519         1324.3136
1356.1987          1405.2550         1420.4497
1449.2760          1549.0514         1641.4881
1711.6557          3057.9711         3107.1208
3167.8896          3175.2371         3228.6672
3239.2296          3257.5844         3261.4967
ZeroEnergy[kcal/mol]  49.85
ElectronicLevels[1/cm] 1
0 2
End

```

```

!-----
!-----5-13-h_ts4-----
Barrier      ts4   r3   R5-1-p4_p4
RRHO
Geometry[angstrom]  16
C   0.747976765    -1.3259770076    2.0489988726
C  -0.100265342    -0.4911468332    1.4492651273
C   0.0227639781    -0.0551382966    0.0570843986
C  -0.4360634384    1.2503128023    -0.440904505
C   0.5929640261    -0.7288179096    -0.9728439641
C  -0.1442549001    1.3628249129    -1.7464412577
C   0.5219770749    0.1034578379    -2.2187995654
H   1.6141661541    -1.718460678    1.5261566616
H   0.6090226712    -1.6253829636    3.0804186215
H  -0.9293226528    -0.0736784688    2.0153196308
H  -0.9176493988    1.9974561758    0.1771006792
H   0.9554892041    -1.747236418    -0.9409943716
H   2.6441876805    -0.1067165547    -0.3310644766
H  -0.344141087    2.2151600925    -2.3807827501
H  -0.064876447    -0.3947563803    -3.0002172038
H   1.5122857121    0.2977636887    -2.6464838973
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  295.9794
WellDepth[kcal/mol]  51.64
WellDepth[kcal/mol]  2.1
End
Frequencies[1/cm]  41
107.9517          160.5239
192.8688          238.9798          279.3359
372.0495          441.1618          557.9944
643.4297          688.5161          750.5309
806.1563          822.5804          921.3312
926.8692          952.5672          967.6229
973.3823          998.2286          1029.4212
1072.8327         1101.5534          1136.1093
1211.4612         1257.0286          1296.6774
1330.7456         1388.6259          1417.8849
1457.0486         1587.7867          1668.8905
1712.8663         3052.7544          3085.0651
3163.9996         3173.3747          3226.3750
3242.7404         3254.2373          3258.2809
ZeroEnergy[kcal/mol]  51.64
ElectronicLevels[1/cm]  1
0  2
End
!-----
End

```

R5_secondary_p4-7

```
Well          r7
Species
RRHO
Geometry[angstrom]  16
C  0.945610569   -1.0733782253   2.0892744343
C  -0.0793796899   -0.4491560141   1.5179772186
C  -0.4017957967   -0.3525066177   0.0440944833
C  -0.7041908525   1.0622514524   -0.4125509063
C  0.6837287279   -0.8321120748   -0.9672843741
C  -0.0490067268   1.3356784623   -1.6022624854
C  0.7350471767   0.2634506828   -2.0003681292
H  1.7031267479   -1.5995701268   1.5191822053
H  1.061521819   -1.0825457557   3.1671446081
H  -0.8043212511   0.0467111135   2.1622572024
H  -1.314068667   -0.9543700339   -0.1086095132
H  -1.3771440722   1.7269632797   0.1131554693
H  0.4486227812   -1.8121579329   -1.3952581924
H  1.6612028107   -0.9371421112   -0.4800441904
H  -0.138438928   2.2665012023   -2.1499343911
H  1.3487130671   0.2234515009   -2.8904880089
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  42
67.2708           108.2254           249.6136
332.6397           467.2041           520.4892
593.1762           604.2744           650.8519
732.6194           808.3302           831.2184
936.9913           938.6147           945.2303
952.8278           1003.6610          1028.4615
1045.6563           1071.7520          1100.7461
1129.0771           1177.8818          1238.3523
1287.3206           1307.8899          1327.0658
1340.5948           1397.9373          1450.0051
1473.3084           1483.0018          1704.2000
2926.8203           3005.3423          3040.1111
3112.9094           3137.1953          3179.0678
3199.8439           3211.5460          3212.6457
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----3-5-c_i4-----
Well          i4
Species
RRHO
Geometry[angstrom]  16
```

```

C 0.0363888173 -1.2558084837 2.8591853063
C -0.2118669693 -0.1963789693 2.0542835317
C -0.0169018177 -0.1847930254 0.6418893511
C -0.3164060435 0.9123545607 -0.1571922848
C 1.4104344922 -0.7562546593 -2.2832590221
C -0.1675098833 1.0580381257 -1.5362334868
C 0.4844251976 0.2060832422 -2.4924154878
H 0.4099791209 -2.1930227466 2.4599187648
H -0.1286167946 -1.2067498327 3.9282033801
H -0.5840189473 0.7227074121 2.5039342989
H 0.3434767856 -1.0998181527 0.1844366571
H -0.7689265509 1.7606190325 0.3541264415
H 1.8208752186 -1.3133923598 -3.1168826793
H 1.8151440389 -0.977926708 -1.3045387366
H -0.6225979626 1.948210815 -1.9614801134
H 0.2153490134 0.4082005508 -3.5276904905
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 42
98.0141 122.2602 163.6553
203.7964 267.6434 365.4250
418.7371 470.7725 596.0793
631.0705 730.7092 800.8518
869.4224 893.6886 899.8913
908.9824 954.5474 976.5221
1008.2946 1026.3932 1086.5136
1177.1419 1188.1954 1262.7298
1306.0890 1317.8375 1324.5971
1437.3126 1449.5261 1469.7842
1524.5572 1598.4157 1621.2308
3113.0688 3118.2458 3122.8047
3135.7645 3147.1280 3151.9453
3171.7981 3226.1968 3235.7960
ZeroEnergy[kcal/mol] 4.65
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c2h3_c5h6_R5-1-p4_p2-----
Bimolecular R5-1-p4_p2
Fragment c5h6
RRHO
Geometry[angstrom] 11
C 1.7739473074 -0.6818466093 -0.7221071247
C 0.7200203695 -1.0943582551 -1.4506225047
C -0.2941048379 -0.0324120696 -1.4821037331
C 0.1452095209 1.0236956202 -0.7726629161
C 1.5088975741 0.7111879701 -0.2184053795
H 2.6777413601 -1.2383555006 -0.515109658
H 0.6186967493 -2.0533819236 -1.9425843223

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H -1.2418186269 -0.1051309279 -2.0003409082
H -0.3745603273 1.9578940938 -0.609861296
H 2.2675009981 1.4252972695 -0.5668910274
H 1.5278529127 0.7618083327 0.87884187
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 27
348.5708 524.1051 681.3317
711.8753 817.0247 818.8020
917.6681 924.4172 953.9591
955.9506 970.7216 1012.6714
1112.1153 1124.7078 1130.0719
1265.2943 1314.9663 1397.2719
1414.9257 1551.9926 1639.1108
3009.5972 3031.2355 3186.6692
3196.7126 3215.2104 3221.8506
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment c2h3
RRHO
Geometry[angstrom] 5
C -2.6815309499 -1.8887734891 -1.1309235268
C -1.725733176 -1.3518528792 -0.4241833636
H -3.0692157655 -1.4200651964 -2.0332260024
H -3.1437000229 -2.8401606701 -0.8523521394
H -1.1628990858 -1.5707617651 0.4715150322
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 9
712.2118 819.4319 921.7170
1046.2369 1391.3607 1651.0507
3037.2336 3133.0072 3234.0563
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 42.96
End
!-----h_c7h8_R5-1-p4_p2-3-----
Bimolecular R5-1-p4_p2-3
Fragment c7h8
RRHO
Geometry[angstrom] 15
C 0.1739997967 -1.5460752179 1.8122391887
C 0.324680931 -0.2480558607 1.5692075473
C 0.7291372666 0.3778604652 0.2539784716
C -0.3525376285 1.2521540983 -0.3524921934
C 1.0763409906 -0.5486182889 -0.8838026578

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C  -0.5545218328    0.8878320403   -1.6301207446
C  0.3404145728    -0.2287387356   -1.9629285648
H  0.340256082     -2.2980345338    1.0494251559
H  -0.1316815966   -1.898276535    2.7910915924
H  0.1383893488    0.4639423486    2.3711994425
H  -0.8602527592    2.0365119332    0.1921908762
H  1.8316078388    -1.3197171321    -0.8190626929
H  1.6052243881    1.0217019264    0.4488942797
H  -1.259254816    1.3360987368    -2.3189316592
H  0.391994327     -0.7034179717    -2.9346653763
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  39
96.6006           162.7769           240.7472
410.1090          530.2283           597.9005
633.7299          702.8545           729.6778
815.8618          843.7614           888.5808
947.4147          953.6961           962.1693
987.9126          1008.7303          1020.2519
1037.3837         1088.8241           1111.2667
1130.4259         1209.6479           1273.9107
1311.0856         1334.3748           1400.3645
1446.8763         1557.3187           1641.3649
1703.5818         2949.9858           3121.5826
3139.7621         3187.0508           3197.1772
3215.6293         3219.3046           3222.2819
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment          H
Atom
Mass[amu]  1
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol]  42.04
End
!-----h_c7h8_R5-1-p4_p3-----
Bimolecular  R5-1-p4_p3
Fragment      c7h8
RRHO
Geometry[angstrom]  15
C  0.7443928714   -1.3490457846    2.1192390514
C  0.0996445535   -0.3097045997    1.5721375373
C  0.114366723    0.0698714649    0.1744554777
C  -0.5402063272   1.1245058925   -0.379086726
C  0.8655128784   -0.6433625597   -0.9280943541
C  -0.2794791736   1.177991565    -1.8144253549
C  0.5348998466    0.16078149    -2.1568642189
H  1.3585019576   -2.0213424081    1.5296606747

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```

H 0.6755628424 -1.5580941948 3.17972883
H -0.5007707266 0.3276416175 2.218356614
H -1.1651757639 1.8260902994 0.1600768602
H 0.5471698061 -1.6886300362 -1.0280933515
H 1.9455396573 -0.6674188552 -0.7360273234
H -0.6852244528 1.9251838977 -2.4843441976
H 0.9079624739 -0.0671847843 -3.1459492301
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 39
124.3028 211.0619 238.3125
366.5748 479.7569 525.8222
618.2448 663.2373 704.7735
826.0168 884.6607 893.9810
910.5914 927.3268 957.2569
958.3030 1013.9583 1026.6553
1035.5369 1123.7193 1134.4806
1214.4226 1255.3239 1321.0912
1340.4518 1393.5409 1419.8632
1447.2796 1553.6099 1628.4275
1679.9293 3021.7172 3047.3312
3126.7072 3139.2148 3187.8486
3199.4255 3220.6212 3221.6809
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 34.2
End
!-----2-3-c_ts1-----
Barrier ts1 r7 R5-1-p4_p2
RRHO
Geometry[angstrom] 16
C 1.0749881854 -0.1335667876 2.1985975693
C 0.0445195079 -0.860063089 1.8448267043
C -0.896439778 -0.3903830416 -0.4368046235
C -0.7045884014 0.9553330961 -0.5532976635
C 0.1287740091 -1.0967032014 -1.2933772729
C 0.4793238694 1.2057841318 -1.3607115041
C 0.9887948974 0.0310859659 -1.794892893
H 1.4179016255 0.7047148228 1.5951455236
H 1.6435477908 -0.3329565083 3.1104580186
H -0.4478813326 -1.7144208304 2.2944714311
H -1.7722803834 -0.8738903959 -0.0309507229
H -1.318217764 1.7239078444 -0.1022860475

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H  -0.365509253   -1.6138301077   -2.1289361006
H   0.6996475048   -1.857057282    -0.7519152191
H   0.8769686537    2.1894442056   -1.577008689
H   1.8696785836   -0.1053300213    -2.4070330807
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  256.1294
WellDepth[kcal/mol]  43.5
WellDepth[kcal/mol]  0.54
End
Frequencies[1/cm]  41
42.1139           84.2214
124.0390          174.7433          258.4607
355.1152          516.9416          686.2089
742.2700          771.6862          811.0192
820.3543          866.2769          891.8190
910.4806          929.7259          934.8301
952.7684          973.1825        1026.6376
1070.4961         1106.0467         1122.7942
1130.3019         1270.6436         1313.1889
1388.9083         1393.6707         1419.1985
1476.8106         1594.9975         1643.0409
3001.7580         3045.0303         3065.3562
3133.1586         3185.8848         3188.1915
3203.2742         3218.0737         3229.8349
ZeroEnergy[kcal/mol]  43.5
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----5-14-h_ts2-----
Barrier      ts2  r7  R5-1-p4_p2-3
RRHO
Geometry[angstrom]  16
C  0.8732065653   -1.127814588   2.0003624413
C  -0.1694407217   -0.4821226247   1.4898268497
C  -0.5059848726   -0.3004894321   0.0296511316
C  -0.7150535063    1.1364044884   -0.400137645
C  0.4167603327   -0.8324959018   -1.0415987157
C  -0.0919778626    1.3480261089   -1.5752884606
C  0.5853243611    0.1233861685   -1.9889085632
H  1.6302561386   -1.5887411382    1.3769388671
H  1.0077908834   -1.202448813    3.0737055322
H  -0.8943851163   -0.0351031572    2.1679032953
H  -1.4743908216   -0.8111014453   -0.1356032418
H  -1.2944524078    1.8501560067    0.1695345806
H  0.7235142787   -1.8661302524   -1.1090174328
H  2.5731553055   -0.6607351231   -0.4026609973
H  -0.0864532404    2.2724321155   -2.1381497454
H  1.1413583993    0.0088463896   -2.9102724659

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Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 349.9455
WellDepth[kcal/mol] 45.5
WellDepth[kcal/mol] 3.46
End
Frequencies[1/cm] 41
85.5927          172.3085
209.5977         241.4124          368.4243
417.9879         530.2727          597.6694
619.2233         695.5232          756.2399
817.6190         844.1994          872.5552
948.2548         952.9856          957.2543
997.1182        1013.4770        1026.5038
1040.2943        1087.7966        1108.7725
1131.6803        1205.6356        1271.6509
1311.4827        1339.3034        1401.9782
1448.7328        1514.7366        1616.5779
1706.5110        2924.6491        3118.9954
3137.3346        3191.2760        3202.4527
3217.8885        3219.1062        3227.7904
ZeroEnergy[kcal/mol] 45.5
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----3-11-h_ts3-----
Barrier      ts3  r7  R5-1-p4_p3
RRHO
Geometry[angstrom] 16
C 0.7906204802 -1.297294226 2.1531183942
C 0.0260532697 -0.3600459352 1.5827925651
C 0.0209054977 0.002019859 0.1718486036
C -0.5510919502 1.1327067782 -0.3628587173
C 0.9138692821 -0.6042055771 -0.8945798925
C -0.1719863893 1.2723355569 -1.7543213317
C 0.6664881547 0.2690294481 -2.0939242192
H 1.4896257814 -1.8988238449 1.5822522844
H 0.7364169765 -1.4933676581 3.2168701848
H -0.6593166172 0.209017795 2.2067760079
H -1.5926892821 -1.1599606764 -0.2314959211
H -1.203011018 1.8108864827 0.173282812
H 0.6982952921 -1.6596099003 -1.086395669
H 1.9655485964 -0.549467106 -0.5833331807
H -0.5190531511 2.0618711554 -2.4080447961
H 1.1085527924 0.0969766503 -3.0657016941
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart

```

```

ImaginaryFrequency[1/cm]  614.0398
WellDepth[kcal/mol]  38.5
WellDepth[kcal/mol]  4.3
End
Frequencies[1/cm]  41
123.7798          208.9852
226.1727          339.0016          399.0880
418.6489          480.3356          532.1840
615.0399          665.0070          703.9257
824.8046          876.5859          879.4042
912.3014          923.1719          957.8865
960.6145          1017.8170         1024.7965
1039.4880          1123.2314         1139.7655
1213.6959          1258.4006         1317.4138
1337.9094          1394.0808         1417.9113
1437.6032          1507.1384         1600.5149
1679.0171          3019.9449         3067.9837
3132.8001          3141.0489         3191.4902
3202.5509          3221.2262         3222.6659
ZeroEnergy[kcal/mol]  38.5
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----3-5-c_ts4-----
Barrier      ts4  r7  i4
RRHO
Geometry[angstrom]  16
C  0.2476801992  -1.4571827296  2.3678584778
C  0.2871709479  -0.3657645153  1.5683756667
C  -0.2443347    -0.2857815606  0.2395562578
C  -0.6529055659  1.0090942436  -0.3699912663
C  1.3174893819  -0.4630336209  -1.2886420158
C  -0.268176524  1.2732874917  -1.6414520088
C  0.5765752204  0.2572748979  -2.2194822585
H  -0.2402010704  -2.3734260961  2.0507636951
H  0.6993192797  -1.4547060284  3.3521252966
H  0.7834961475  0.5282313837  1.9445979859
H  -0.8335618622  -1.1446289235  -0.0862907236
H  -1.2982931308  1.6841614082  0.1861644733
H  1.6875644977  -1.458577814  -1.5209693826
H  1.9036428563  0.0685282924  -0.5501206682
H  -0.645292552  2.1234554815  -2.2001550571
H  0.39905459    -0.1088631091  -3.2260530421
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  731.8116
WellDepth[kcal/mol]  34.7
WellDepth[kcal/mol]  30.05
End

```

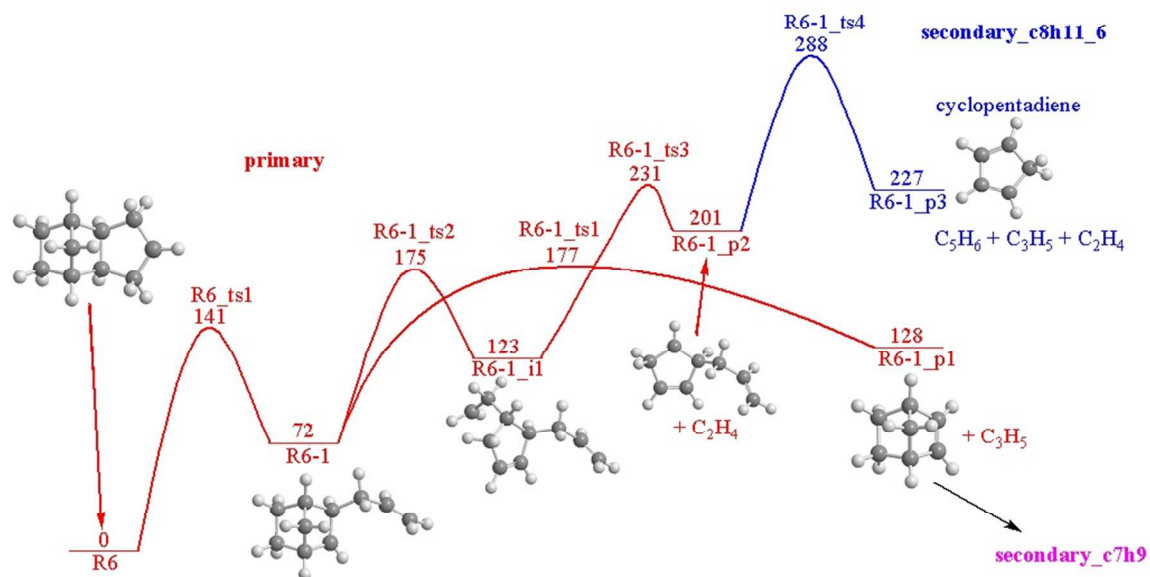
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Frequencies[1/cm]  41
125.3283          143.8725
214.8781          318.3345          384.1060
507.4414          516.9680          626.7752
673.1175          724.6405          749.8122
784.9361          861.9374          875.4917
924.6789          962.5317          972.8074
1008.2173         1013.2648         1058.3420
1073.0786         1153.7992         1199.4886
1233.8234         1286.9741         1301.9104
1371.0042         1416.3653         1459.2962
1512.8056         1578.3566         1587.5916
3084.3543         3111.8352         3118.8962
3131.1521         3138.3670         3152.0686
3174.6925         3200.0992         3220.9442
ZeroEnergy[kcal/mol]  34.7
ElectronicLevels[1/cm]  1
0  2
End
!-----
End

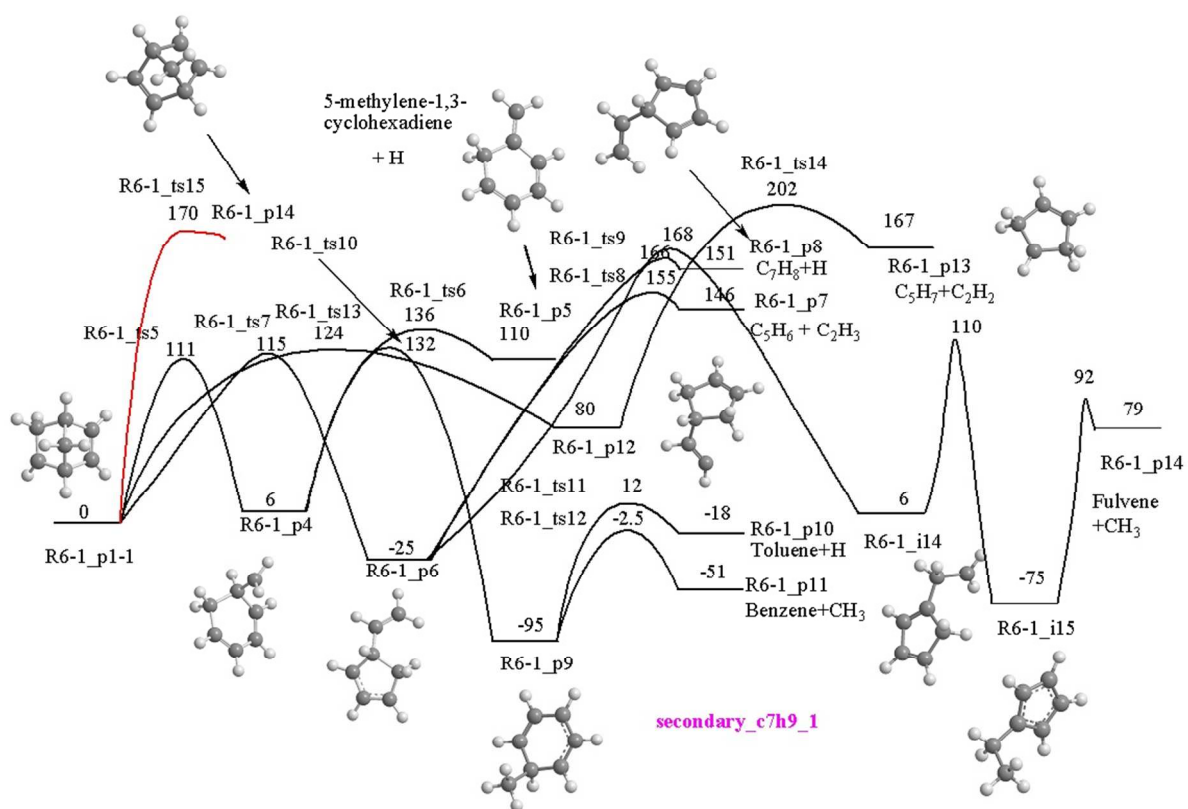
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Cartesian coordinates and vibrational frequencies of stationary points in R6 channel

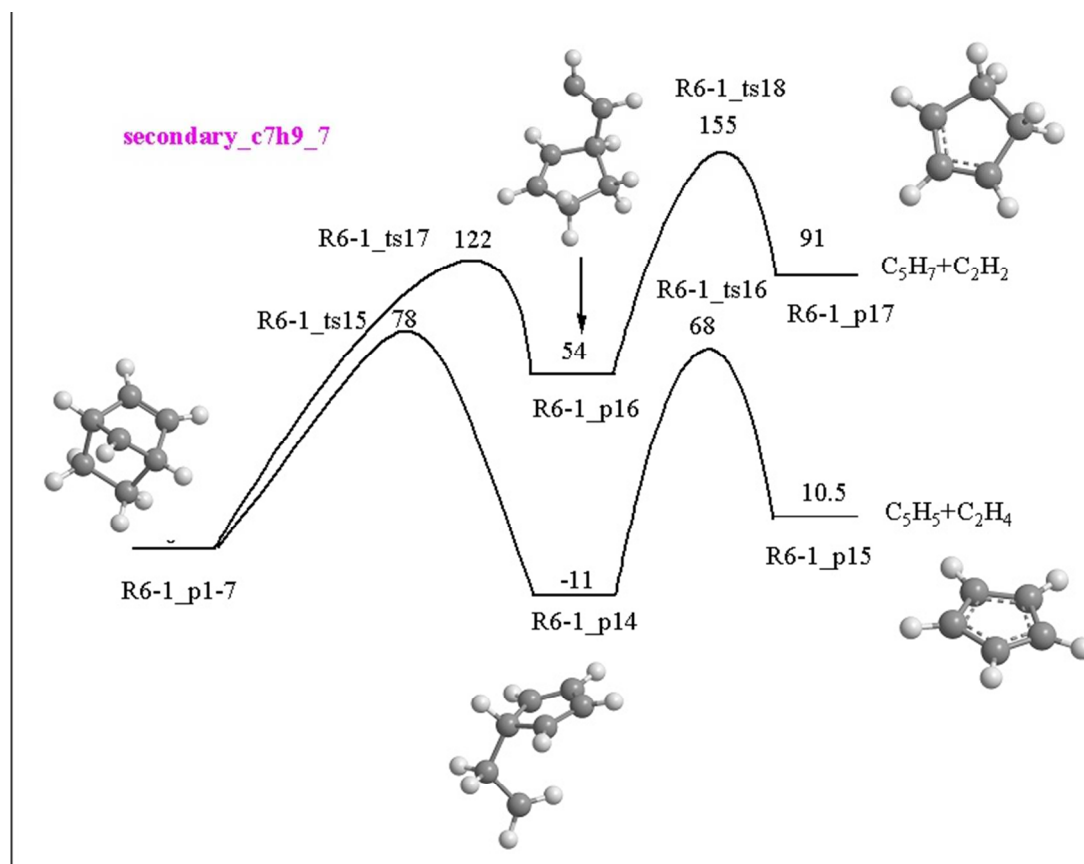
Please refer to the following schemes for the notation of stationary points involved in R6 channel. Cartesian coordinates and vibrational frequencies of the stationary points are given below in the form of the corresponding fragments of the MESS input file.



Scheme S6. R6 channel.



Scheme S7. R6_secondary_c7h9-1.



Scheme S8. R6_secondary_c7h9-7.

R6_primary

```
Well          R6
Species
RRHO
Geometry[angstrom]  25
C   -0.7119290078    0.3393298588    2.2522094092
C   -0.0517136933   -1.0786123749    2.2510633589
C    0.8810713836   -1.0303685097    1.0183360513
C    0.0057603827   -1.0585401561   -0.2577590151
C   -0.6611427541    0.373705601   -0.2566152494
C   -0.0754088044    1.0237818102    1.0199939242
C    1.3541029518    0.4396239938    1.0489443514
C    0.7854937928   -1.1947525094   -1.5922999113
C   -0.2643642515    1.0598828128   -1.590495551
C    0.4495791819    0.021215345   -2.3897786707
H   -0.4688493429    0.8855116925    3.1676027883
H   -1.8017580006    0.2975925423    2.1782415433
H   -0.7852035566   -1.885682731    2.176421186
H    0.523286064   -1.2453859845    3.1658878484
H    1.664462428   -1.79108526    1.0275445047
H   -0.7457524921   -1.848539694   -0.1857513199
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H  -1.7494082328    0.3069156988   -0.1840017198
H  -0.1533690019    2.1129489251    1.0306712059
H   1.9609327953    0.7228905479    0.1850352526
H   1.9060318954    0.695886489    1.9578616989
H   0.5251242573   -2.1219291723   -2.1205810944
H   1.8700415879   -1.2689680343   -1.404406682
H   0.3769743794    1.9374696498   -1.4018614269
H  -1.141881589    1.4580390684   -2.1177259802
H   0.7864866269    0.1789243909   -3.4078835022
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 69
39.3695          108.0334          254.7470
257.4276          322.5084          384.9275
394.7616          497.6710          530.1222
689.4469          714.7634          729.5326
764.9459          796.9032          825.5546
836.6991          887.0684          890.4478
907.4772          925.1308          934.6003
942.5751          963.1817          963.6286
1014.6507         1019.9342         1044.4642
1053.0720         1058.4408         1081.0288
1129.1098         1139.2769         1146.4282
1174.3685         1199.8383         1211.7259
1230.3315         1248.9287         1267.2486
1288.7569         1301.8759         1303.6067
1306.6620         1318.2505         1324.9008
1345.9345         1352.1147         1360.6079
1375.4458         1471.0227         1474.1907
1491.6578         1503.7395         1523.4335
2928.7294         2931.1255         2988.4242
2988.6814         3033.2386         3040.9327
3043.9772         3044.8654         3060.2528
3064.0769         3073.7437         3080.2970
3083.3976         3087.2675         3177.0521
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c10h15_R6-1-----
Well          R6-1
Species
RRHO
Geometry[angstrom] 25
C  -1.0932632231    0.3085323487    2.2203781872
C  -0.3961892221   -1.0449129025    2.5765345584
C   0.8365870235   -1.0575572314    1.6134003146
C   0.3139991627   -1.2055099652    0.2151601034
C  -0.3598235126    0.086469195   -0.1757310689

```

C	-0.172018373	0.9140999322	1.129797381
C	1.2155875987	0.4451129456	1.6208100584
C	0.9137290954	-0.5382792793	-3.4882165707
C	0.2317137858	0.7646365064	-1.4430666831
C	-0.0220642299	-0.021560099	-2.6969625492
H	-1.1421005588	0.9668616914	3.0916371742
H	-2.1157107138	0.1713494614	1.8590549831
H	-1.043773679	-1.909987682	2.4214443144
H	-0.0638205977	-1.0622218418	3.6193567272
H	1.6135612395	-1.7662647628	1.9030034324
H	0.24201807	-2.1341228956	-0.3359230254
H	-1.4328685389	-0.0629062412	-0.3717576159
H	-0.2989978882	1.9892803381	0.9898928668
H	2.032401287	0.6849395577	0.9369355948
H	1.4650552888	0.8213482444	2.6172665031
H	0.6592373662	-1.1002917352	-4.3800809046
H	1.9710383795	-0.4143840253	-3.2735903897
H	1.3062183796	0.9253594567	-1.3168205279
H	-0.2355680995	1.7540761292	-1.5392691453
H	-1.0702030401	-0.1758531455	-2.952846718
Core RigidRotor			
SymmetryFactor 1.0			
End			
Frequencies[1/cm] 69			
71.4602	77.0604	130.6202	
192.2793	260.0251	284.7261	
308.3827	380.9507	448.0425	
470.7205	505.2442	633.6215	
647.7625	766.1301	776.7264	
813.8201	841.1009	863.2078	
879.0546	918.0518	933.5546	
939.5626	942.1476	952.2759	
956.6573	959.8196	1014.3111	
1023.2176	1034.3948	1038.7506	
1061.5995	1108.0244	1136.2685	
1144.8078	1170.5936	1198.3511	
1221.1345	1240.7058	1257.4963	
1280.2133	1285.4671	1299.3838	
1306.3921	1326.5364	1329.3442	
1345.4229	1353.8511	1361.4013	
1451.6970	1483.2140	1491.8757	
1499.3336	1519.1341	1706.2252	
2956.3812	2995.9095	3028.5508	
3040.9585	3044.0632	3062.7617	
3070.2613	3080.2997	3088.7444	
3091.1158	3093.5423	3109.3551	
3125.6238	3200.1630	3206.2567	
ZeroEnergy[kcal/mol] 17.21			
ElectronicLevels[1/cm] 1			
0	2		
End			
End			

```

!-----
!-----c10h15_R6-1_i1-----
Well          R6-1_i1
Species
RRHO
Geometry[angstrom]  25
C  -1.2283670607    0.7028732201    2.2798559254
C  -1.6520666993   -0.639428527    2.7691193939
C   1.5993889069   -1.1211322686    1.2834563966
C   0.8190512848   -1.254538844    0.2136300347
C  -0.1547259853   -0.1109533252    0.0552185844
C   0.0349220947    0.7196638874    1.367046078
C   1.2949811368    0.1294620761    2.0661847846
C   0.74151587     -0.2772582493   -3.446393716
C   0.0946297962    0.7242404429   -1.2268875486
C  -0.1590234541   -0.0345895478   -2.498136296
H  -1.0231612603    1.3595044641    3.1345688791
H  -2.0475286708    1.1664005587    1.7161489728
H  -2.3230707432   -1.2620926447    2.1904113017
H  -1.2123545524   -1.0771875411    3.6568296003
H   2.3806867753   -1.8159886199    1.5722181198
H   0.8734976934   -2.0699746667   -0.4982541661
H  -1.1827126208   -0.4939256245   -0.0032811241
H   0.2130457083    1.7679707014    1.1079892559
H   2.1406200882    0.8277077589    2.0403212177
H   1.1126908051   -0.0842364842    3.1258102148
H   0.4895533336   -0.8326291033   -4.343050306
H   1.7651925778    0.0751290317   -3.3610380687
H   1.1210103599    1.1067390519   -1.217876253
H  -0.5733408906    1.5957420461   -1.194312204
H  -1.1734184935   -0.411443793   -2.6281750772
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  69
23.7788           64.0790           64.6344
86.5964           125.8549          180.8774
205.4935          271.4591          288.2459
366.8964          422.0339          448.7518
504.0363          598.2986          628.5862
710.9785          743.4201          762.5578
794.7016          824.3258          867.2449
933.3336          943.1243          946.8241
969.3033          974.1021          989.4574
999.2700          1029.5863         1044.1087
1052.2802         1079.1648         1114.8338
1136.0248         1142.8492         1185.3607
1235.6097         1247.8259         1267.7092
1287.0141         1303.1620         1321.6654
1326.9436         1339.4572         1349.4815
1379.0910         1392.5124         1451.6567
1466.7328         1481.3816         1487.0611

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1491.3763          1685.6516          1706.1488
2988.9600          2993.5457          2994.8388
3006.5914          3027.1662          3033.1534
3039.8842          3049.8724          3109.3759
3125.4965          3138.5127          3165.7657
3192.9208          3206.8798          3236.3354
ZeroEnergy[kcal/mol] 29.40
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----c3h5_c7h10_R6-1_p1-----
Bimolecular      R6-1_p1
Fragment          c7h10
RRHO
Geometry[angstrom]  17
C  -1.0586145498    0.3649669683    0.6821024869
C  -0.3343347059   -0.976959028    1.0141185505
C   0.8622844197   -0.9860148367    6.74294E-5
C   0.2422157964   -1.1287228019   -1.3828424652
C  -0.3783336062    0.0209984884   -1.6672918999
C  -0.1845778645    0.9535215373   -0.4797316145
C   1.2247789777    0.517297255   -0.0160577023
H  -1.0542512362    1.0407621565    1.5416305968
H  -2.0967528448    0.2229363858    0.377011182
H  -0.9783426095   -1.8491862622    0.8898101269
H   0.0380029038   -0.982412252    2.0421475438
H   1.6565915266   -1.6898352584    0.2480760266
H   0.2192444026   -2.0459847115   -1.95847769
H  -1.0100917926    0.2314055958   -2.5216089197
H  -0.3431232548    2.0151206029   -0.6685939137
H   2.0039837621    0.7584542099   -0.7417532339
H   1.5000926752    0.9093239507    0.9680624962
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  45
261.0148          383.1124          478.7763
485.5499          676.8263          726.6779
775.3439          800.9555          819.3468
837.2773          880.0754          908.0001
917.7600          940.4461          954.2970
963.8291          972.6069          1037.9626
1053.6840         1113.0512          1140.1114
1147.6029         1187.3603          1189.8654
1236.0884         1281.8249          1290.0623
1300.6989         1306.2256          1326.8517
1361.3279         1492.6393          1492.9381
1515.3672         1634.6807          3036.4419
3039.5294         3052.1235          3081.7005
3095.2965         3098.5685          3100.6431

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3103.3924          3178.0114          3203.1123
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
Fragment      c3h5
RRHO
Geometry[angstrom]      8
C  0.0  0.0  0.4414918248
H  0.0  0.0  1.5297451707
C  0.0  1.2274571769  -0.1957824309
C  0.0  -1.2274571769  -0.1957824309
H  0.0  2.1546553362  0.3627527557
H  0.0  -2.1546553362  0.3627527557
H  0.0  1.2960812234  -1.2782433226
H  0.0  -1.2960812234  -1.2782433226
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  18
429.8649          531.6773          551.3484
785.3716          810.5065          936.5863
1012.9503         1037.0010         1207.5850
1270.2294         1423.3954         1511.2262
1517.2794         3126.8472         3133.4950
3139.8670         3231.6020         3234.4382
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  2
End
GroundEnergy[kcal/mol]  30.59
End
!-----c2h4_c8h11_R6-1_p2-----
Bimolecular      R6-1_p2
Fragment      c8h11
RRHO
Geometry[angstrom]      19
C  1.0300728611  -0.9543190865  1.9428526217
C  0.334599191  -1.051034355  0.8103176113
C  -0.6607753164  0.081558399  0.6448439888
C  -0.4286500272  0.8801438081  1.8958452402
C  0.6244086514  0.253998621  2.7587331049
C  0.0460078591  -0.154925814  -2.8970525405
C  -0.4745202137  0.8990493903  -0.6698126257
C  -0.8010177318  0.1129640735  -1.9070547883
H  1.798531061  -1.6474682435  2.2651392068
H  0.4511409723  -1.8307149033  0.0674412704
H  -1.6901054179  -0.3190990487  0.617799029
H  -0.9766246738  1.7783823122  2.1505649419
H  1.4757065235  0.9243072613  2.9602121313
H  0.2446679013  -0.0315987138  3.753896333
H  -0.2562777971  -0.7294080851  -3.7656862172

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H  1.0732829898    0.1967171566   -2.8764840353
H  0.5525070716    1.2734033471   -0.7167091179
H  -1.1353217884    1.7734222882   -0.613005446
H  -1.8216531158   -0.2637574073   -1.9719387082
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  51
71.7239              85.2509              130.4701
211.1848             303.2548              324.8843
379.2208             427.3658              501.7299
625.9266             723.9821              759.7416
778.3109             866.9830              913.9047
929.4861             934.1191              938.4850
944.5743             973.0509              992.3585
1028.6668            1034.0049             1057.5922
1109.5010            1130.6019             1132.2036
1224.4974            1248.2528             1285.9975
1301.8592            1322.7452             1325.8822
1335.9831            1390.7712             1450.1638
1460.8642            1481.5690             1672.6710
1704.9764            2911.6504             2943.5137
2951.3456            3005.9342             3061.9706
3109.9050            3125.8702             3174.8880
3195.2167            3201.5706             3207.1048
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0  2
End
Fragment              c2h4
RRHO
Geometry[angstrom]    6
C  0.0    0.6634900906    0.0
C  0.0   -0.6634900906    0.0
H  0.0    1.23462754   -0.9225248038
H  0.0    1.23462754    0.9225248038
H  0.0   -1.23462754    0.9225248038
H  0.0   -1.23462754   -0.9225248038
Core  RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm]  12
834.2929              972.9227              974.1218
1066.8559             1238.5875             1379.4650
1472.0483             1691.5384             3121.2072
3136.3255             3192.3844             3220.8390
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0  1
End
GroundEnergy[kcal/mol]  54.25
End

```

```

!-----c10h15_R6_ts1-----
Barrier      R6_ts1  R6  R6-1
RRHO
Geometry[angstrom]  25
C  -0.8147399517   0.3568272485   2.342941974
C  -0.1979369287  -1.0788170869   2.4104345729
C   0.7788532624  -1.0933593283   1.1925436222
C  -0.089622304   -1.0887628987   -0.047457282
C  -0.661161882   0.3283300848  -0.1694559568
C  -0.1077146808   0.9931338365   1.1202099382
C   1.2980887583   0.3615139403   1.2267723914
C   0.9993489039  -1.0508117318  -2.0282223731
C  -0.1897763302   1.0106709423  -1.5094181967
C   0.1102402817  -0.1056695856  -2.4666287517
H  -0.5961155892   0.9211380292   3.2533858231
H  -1.9011093055   0.3420197856   2.2230880043
H  -0.9501091189  -1.8678239266   2.3417526738
H   0.3551274155  -1.232134699   3.3426162497
H   1.5253731509  -1.888112542   1.2398046686
H  -0.7236171221  -1.9473727399  -0.2439550226
H  -1.7563763053   0.3183211119  -0.1585373262
H  -0.1468349307   2.084254995   1.1033668417
H   1.959426137   0.6113698095   0.3947340699
H   1.8077035105   0.612065911   2.161253116
H   1.088580096   -2.0108449063  -2.5276520419
H   1.8583426613  -0.7693587067  -1.4279902087
H   0.7107665281   1.6036877426  -1.3111581657
H  -0.9489941028   1.7009417566  -1.883791624
H  -0.6060831538  -0.3456280418  -3.2466569965
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  507.6033
WellDepth[kcal/mol]  33.7
WellDepth[kcal/mol]  16.49
End
Frequencies[1/cm]  68
121.1275          160.1360
259.4620          276.4294          323.3931
384.9795          460.2764          477.5802
537.1137          648.8494          661.1690
739.9116          767.2809          775.1614
808.4394          833.9406          856.3991
882.2232          904.7071          912.6572
921.7281          929.4720          938.3498
947.3289          956.6127          969.6065
992.4432          1024.3162         1039.8631
1047.0743         1085.7914          1137.5272
1149.0564         1176.9563          1200.9198
1213.0277         1231.8866          1242.8211
1262.3153         1282.6313          1287.2217

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1296.4470          1304.1709          1311.4542
1336.8823          1342.3618          1348.3249
1417.5982          1489.5375          1491.4928
1502.0612          1519.0016          1552.8207
3014.2357          3021.0114          3027.1868
3042.1232          3046.8464          3067.6313
3076.6103          3078.6172          3082.4017
3087.4356          3093.0589          3117.2568
3149.5147          3152.7026          3193.3212
ZeroEnergy[kcal/mol] 33.70
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c10h15_R6-1_ts1-----
Barrier          R6-1_ts1  R6-1  R6-1_p1
RRHO
Geometry[angstrom] 25
C 0.1774473617 0.7417021374 2.1699734503
C -0.7057611142 -0.4534268471 2.6487441844
C -0.669854564 -1.4204189102 1.4135575825
C -1.4096811705 -0.6904035221 0.3152143436
C -0.5953655856 0.329256797 -0.1500220022
C 0.6431949541 0.2949973912 0.7459721797
C 0.7970077781 -1.2264779982 0.9621000614
C 0.7072347521 2.1098022329 -3.08746462
C 0.0772799584 -0.1029195382 -2.1774550393
C 1.0172427219 0.9179159311 -2.5234700581
H 1.0413018713 0.8828395553 2.8251220118
H -0.3691743688 1.6864719102 2.1397699551
H -1.7241959752 -0.1547869496 2.9035342712
H -0.2732434826 -0.9434627768 3.5264212171
H -0.9968119257 -2.4372718268 1.6319200574
H -2.4535889367 -0.841196898 0.0692600711
H -0.979480892 1.2649447597 -0.5395145441
H 1.5103449827 0.836399099 0.3695255678
H 1.0440139239 -1.7739828273 0.0514040575
H 1.5202628331 -1.4793129018 1.7424665885
H 1.4654953738 2.8555636944 -3.2926407625
H -0.3123605693 2.3536096136 -3.3697988951
H -0.9146451583 -0.0496069575 -2.6135864737
H 0.4441278595 -1.1081930471 -2.0175033491
H 2.0584903722 0.7309788789 -2.2674888554
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 558.0886
WellDepth[kcal/mol] 25.09
WellDepth[kcal/mol] 11.71
End
Frequencies[1/cm] 68

```

35.7021	85.7309	
140.2775	156.2711	239.1388
267.3051	385.1955	425.9867
445.8333	484.5194	631.5581
647.4340	705.2919	732.3820
778.8021	788.9643	817.2592
833.5033	843.0519	862.8807
878.1514	909.1985	927.9635
937.7530	952.1667	962.1148
975.3381	1004.3901	1008.1544
1034.1692	1034.6438	1048.1348
1086.5042	1137.4376	1141.3926
1182.9520	1194.3494	1213.6053
1234.9417	1279.7841	1286.1041
1297.2026	1300.4080	1304.1440
1326.7988	1356.4238	1422.2465
1441.4547	1490.6155	1493.3658
1500.3756	1519.4733	1586.8849
3032.3422	3045.8922	3051.0635
3077.6922	3094.5180	3095.3053
3104.3825	3108.5253	3122.1208
3128.4359	3132.7351	3161.4223
3192.2466	3218.1850	3224.7246
ZeroEnergy[kcal/mol] 42.30		
ElectronicLevels[1/cm] 1		
0 2		
End		
!-----		
!-----c10h15_R6-1_ts2-----		
Barrier	R6-1_ts2	R6-1 R6-1_i1
RRHO		
Geometry[angstrom] 25		
C	-1.1158117596	0.5049128369 2.6645307771
C	-0.7113622723	-0.8658718718 3.1603931
C	1.0862579047	-0.9732234581 1.8192862078
C	0.407608552	-1.1492201438 0.6394113084
C	-0.3179796589	0.1252205911 0.2641445996
C	-0.1269150649	0.9746301177 1.5578413757
C	1.2520063322	0.5183981845 2.0693015398
C	0.9261085273	-0.5048588396 -3.0510582688
C	0.2336321591	0.8098319219 -1.0168606342
C	-0.0141069311	0.0054673654 -2.2608764917
H	-1.0851595085	1.2315648078 3.4834433744
H	-2.1400165325	0.5049294497 2.2758103838
H	-1.2962240865	-1.72638503 2.8579746912
H	-0.2655200058	-0.9513305465 4.1465893764
H	1.7196521176	-1.7254277946 2.2750760699
H	0.2679657387	-2.0927070577 0.1279491663
H	-1.3878475464	-0.0649067781 0.0933962064
H	-0.2159110408	2.0479512844 1.3702187216
H	2.0773909773	0.9241388061 1.4736873096
H	1.4298410526	0.7842463205 3.1136622197

```

H  0.6766169557   -1.0824490307   -3.9343135191
H  1.9821683555   -0.3603495146   -2.8433307421
H  1.3055923207    0.9989800262   -0.9051825527
H  -0.25926748    1.7860368035   -1.1167263041
H  -1.0609541061   -0.1698174502   -2.5081479149
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  517.5777
WellDepth[kcal/mol]  24.62
WellDepth[kcal/mol]  12.43
End
Frequencies[1/cm]  68
63.5684          72.0584
118.3103         190.7726         207.2828
298.9072         349.7712         388.4220
438.7460         480.9501         541.7555
575.3288         640.6974         710.5731
752.7804         777.9077         801.1886
818.5919         862.3256         869.5432
907.4964         926.8333         934.3728
942.2178         956.5525         976.5115
992.4327         1014.6911        1022.7115
1035.7852        1049.7050        1094.8951
1102.5718        1127.9048        1155.5304
1199.0243        1233.8446        1246.7291
1270.3615        1286.1994        1302.0962
1316.1951        1330.2667        1335.3293
1365.9212        1375.3811        1450.1995
1465.5070        1476.2421        1483.1426
1494.0042        1510.6315        1705.9780
2972.3385        2998.6964        3012.6544
3026.5066        3049.2809        3059.5970
3062.5789        3078.3880        3110.2010
3118.2282        3125.9508        3177.1316
3202.5993        3206.7775        3208.4386
ZeroEnergy[kcal/mol]  41.83
ElectronicLevels[1/cm]  1
0  2
End
!-----c10h15_R6-1_ts3-----
Barrier      R6-1_ts3  R6-1_i1  R6-1_p2
RRHO
Geometry[angstrom]  25
C  -1.2544183008   0.7145061319   2.6189527705
C  -1.4500061547  -0.5929940629   2.945819454
C  1.9323348282   -0.9405262921   1.3511553448
C  1.1602862281   -1.0593180671   0.2720355991
C  0.2873209733   0.1584964405   0.0512263373
C  0.5475872572   0.9731946503   1.3065667768
C  1.7110011927   0.3717771033   2.0657647652

```

C	1.1907179091	-0.198972839	-3.4376171043
C	0.6284643911	0.9301963592	-1.2582293903
C	0.311147003	0.1539142724	-2.5043468941
H	-0.8126126058	1.3929796472	3.3409871162
H	-1.8681085597	1.1794999477	1.854690605
H	-2.0254468103	-1.2570984449	2.311005324
H	-0.965227444	-1.0419462244	3.8052743343
H	2.6481620998	-1.6802924082	1.6912317716
H	1.1542450376	-1.9068876666	-0.4026815242
H	-0.7707159402	-0.1353677757	-0.020698904
H	0.4414444051	2.0531869827	1.2613113017
H	2.6081460755	1.0088936183	2.0245751921
H	1.4984784371	0.2318350581	3.1344993679
H	0.8945925669	-0.7601152806	-4.3170016904
H	2.2407776236	0.0659394237	-3.3568909433
H	1.686165771	1.211872001	-1.250442674
H	0.0453163685	1.8604558844	-1.2575889766
H	-0.7319673524	-0.1368504592	-2.6271269593

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 445.3763

WellDepth[kcal/mol] 25.81

WellDepth[kcal/mol] 0.96

End

Frequencies[1/cm] 68

48.7434	54.6615	
71.3335	88.5118	139.7722
177.7813	201.2280	255.0732
323.2293	373.1346	417.0441
429.6132	505.5439	632.3344
716.7174	727.5406	777.1436
784.0967	820.0543	840.3009
867.4735	890.4390	927.2597
938.8841	944.6219	956.1353
970.0911	987.1359	998.6613
1011.9015	1033.8378	1035.8344
1080.0579	1113.1344	1131.0827
1159.9680	1228.3551	1239.2507
1256.6616	1271.9673	1288.9185
1306.3053	1323.6155	1329.7914
1338.3725	1385.4379	1449.5883
1463.8936	1466.7517	1480.9416
1567.3423	1674.7175	1704.8329
2960.1601	2966.0006	2991.1750
3000.0800	3056.8103	3110.6053
3115.2158	3126.1965	3134.4621
3144.7192	3172.2464	3191.5376
3198.5036	3207.5355	3223.1765

ZeroEnergy[kcal/mol] 55.21

R6_secondary_c7h9-1

```
!-----R6-1-pl_r1-----
Well          r1
Species
RRHO
Geometry[angstrom]  16
C  -0.8812774816    0.5666743775    0.8353213473
C  -0.2508177293   -0.7626095928    1.1668047715
C   0.8893575521   -0.8377829998    0.0861829201
C   0.1845728119   -0.9384067941   -1.2611059537
C  -0.4050520784    0.2401199465   -1.4967873552
C  -0.0851677414    1.1636373132   -0.3102694562
C   1.3337103044    0.6463274331    0.047731116
H  -1.8943549995    0.8515081665    1.0887424864
H  -0.9455330109   -1.607170972    1.098480241
H   0.1739461012   -0.7786410086    2.1799949819
H   1.6573126084   -1.583186767    0.2898052384
H   0.0871395252   -1.8471589776   -1.8414947637
H  -1.0927847848    0.4864056012   -2.2961026098
H  -0.211879136    2.2315282049   -0.4818212471
H   2.0666512542    0.8480044353   -0.7358370595
H   1.6965098045    1.0188366336    1.0098683427
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  42
278.3046          347.0669          457.3689
483.1699          509.2301          676.0790
727.4704          778.9181          795.0002
845.4489          887.7345          897.3475
902.3390          930.7297          943.3297
952.3409          983.9483          996.2481
1028.2289         1104.7838         1119.2608
1141.4054         1174.3028         1198.3049
1248.2925         1273.2131         1281.5501
1301.9558         1320.7609         1347.5068
1472.7301         1496.4806         1616.2234
2987.3669         3030.2215         3043.2387
3100.4715         3104.1693         3109.3711
3182.1734         3195.0592         3207.3309
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----R6-1_ip4-----
Well          ip4
Species
RRHO
```

```

Geometry[angstrom] 16
C -1.1224184662 0.2850566358 1.1218849076
C -0.2104910019 -0.8389523712 1.5454297432
C 0.8157264013 -1.2153227279 0.770274747
C 1.1032943568 -0.5127311804 -0.4803035541
C 0.5156315291 0.6594214781 -0.7669157617
C -0.4167797899 1.336645182 0.2334426221
C 0.4220116184 2.3087899616 1.0063596816
H -1.5607055476 0.7814041381 1.9928230221
H -1.9637028016 -0.1478094344 0.5597679573
H -0.4376749994 -1.3729083048 2.4625477362
H 1.4422509172 -2.0556360508 1.0506197289
H 1.8193892993 -0.9490597296 -1.1693101399
H 0.7612846831 1.2016735375 -1.6739774753
H -1.1824467501 1.892404551 -0.3166267077
H 1.0902337606 1.9450744306 1.7783302975
H 0.5659517909 3.3204598843 0.6463771953
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 42
135.7173 182.2240 212.1440
325.9045 370.9277 509.3749
560.1975 571.8365 606.3248
697.2224 782.6456 787.4319
863.4393 924.7867 933.6306
970.3971 981.4608 987.9108
1027.4967 1088.7348 1101.0817
1174.6524 1201.1893 1242.5107
1290.0939 1333.6574 1360.0528
1389.8511 1435.3291 1453.5177
1469.2316 1619.8724 1693.5886
2974.8911 3035.4026 3054.1751
3132.8086 3146.9402 3154.3514
3169.7706 3178.2692 3238.3411
ZeroEnergy[kcal/mol] 1.43
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----R6-1_ip6-----
Well ip6
Species
RRHO
Geometry[angstrom] 16
C -1.1597413622 0.4122124829 0.901044743
C -0.9715218792 0.0585671943 2.1683900769
C 1.7402256134 -0.6471583368 -1.1032504028
C 0.6592569244 -0.7779826195 -1.9619097281
C -0.4534012416 -0.1145493415 -1.4706894488
C -0.1143192219 0.5982274816 -0.1751243265

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C 1.3354383556 0.1137183272 0.1326186077
H -2.1765362737 0.6192847003 0.5697277592
H -1.8080922728 -0.0289215552 2.8523631598
H 0.0096750333 -0.153141706 2.5784440664
H 2.7234513039 -1.0729390127 -1.2531748097
H 0.681143875 -1.3271788056 -2.8958680291
H -1.4242452985 -0.0579369288 -1.9453805336
H -0.0848778893 1.6806690428 -0.3878380529
H 2.0107427867 0.9441926099 0.3632827812
H 1.3551345469 -0.5489785329 1.0068771375
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 42
67.2446 108.2154 249.6470
332.6191 467.2047 520.5028
593.1888 604.2720 650.8509
732.6422 808.3350 831.2075
936.9858 938.6091 945.2277
952.8162 1003.6557 1028.4573
1045.6468 1071.7518 1100.7404
1129.0802 1177.8872 1238.3486
1287.3325 1307.8963 1327.0581
1340.5977 1397.9337 1449.9994
1473.3068 1482.9981 1704.1760
2926.8500 3005.3738 3040.0953
3112.9069 3137.1983 3179.0681
3199.8451 3211.5470 3212.6479
ZeroEnergy[kcal/mol] -5.98
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----R6-1_ip9-----
Well ip9
Species
RRHO
Geometry[angstrom] 16
C -1.5153030016 0.3620454311 0.6525141815
C -0.4357640907 -0.3659289629 1.0558075822
C 0.6982942492 -0.7194947732 0.1322982066
C 0.4717585985 -0.2167817031 -1.2676759961
C -0.6269396073 0.5080439319 -1.6219168663
C -1.641237351 0.8187689224 -0.6827495617
C 2.0606913431 -0.2307786968 0.6958041982
H -2.2984191473 0.5970246955 1.3666268587
H -0.3613647882 -0.707575558 2.0837825843
H 2.0742034865 0.8589739553 0.7710345972
H 0.7775960566 -1.8221403451 0.0924923139
H 1.2355963015 -0.4451222095 -2.0048346171
H -0.7313840635 0.8545598191 -2.645372368

```

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H -2.5063272051 1.3964483317 -0.9835605626
H 2.8820798963 -0.5421229987 0.0442198733
H 2.2388523238 -0.6478348398 1.6910425735
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 42
94.0113 235.5013 283.4476
381.0001 427.3975 534.0457
593.1611 612.5367 674.2754
743.8710 782.2625 803.1320
930.3125 954.7247 968.6102
974.6338 990.3870 1033.6015
1053.3709 1085.7894 1121.3693
1176.3810 1197.7845 1281.5361
1309.9029 1356.4496 1394.8946
1406.5654 1456.0573 1493.2542
1500.5822 1542.0611 1603.0101
2888.3307 3021.9368 3088.2993
3100.4706 3144.4737 3145.1899
3163.4699 3164.5471 3192.2295
ZeroEnergy[kcal/mol] -22.7
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----R6-1_ip12-----
Well ip12
Species
RRHO
Geometry[angstrom] 16
C -0.7900062636 0.7256073353 1.316441243
C -0.4100298958 -0.7140806881 1.0739424737
C 0.6914713721 -0.6231558757 -0.0352611896
C 0.1523607174 -1.1038450771 -1.3680564713
C 0.056093894 -0.4296045297 -2.4840053881
C 0.0402948662 1.5746997821 0.716833397
C 1.1335796063 0.8680119275 -0.0450746971
H -1.6357308239 1.0098752297 1.9323443583
H -1.2609472831 -1.3267438746 0.7568768422
H -0.019539736 -1.1757225213 1.9897337087
H 1.5305667409 -1.2753942991 0.2260450423
H -0.1985652696 -2.1445848249 -1.3650113126
H -0.2911485564 -0.5886110458 -3.4933599476
H -0.0282356766 2.6552748742 0.7725294456
H 1.2490321599 1.2459116463 -1.0656395311
H 2.1031371483 1.0004469411 0.4511750267
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 42

```

54.7107	103.4083	252.6183
353.7257	386.9294	515.1083
618.7529	676.9675	743.3131
762.7408	786.5750	828.3954
856.7589	899.4766	953.4773
973.0314	976.3684	995.6685
1039.8928	1083.0755	1130.5435
1184.8257	1192.6786	1230.2585
1263.9905	1311.4288	1327.4868
1343.2923	1375.9924	1482.8181
1491.1514	1670.6067	1686.5090
2995.1672	3002.1879	3006.0804
3035.1155	3040.0630	3046.8549
3166.3220	3191.1013	3244.4342
ZeroEnergy[kcal/mol] 19.2		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----h_c7h8_R6-1_p5-----		
Bimolecular R6-1_p5		
Fragment c7h8		
RRHO		
Geometry[angstrom] 15		
C -1.057176651	0.0173953652	0.6864071322
C -0.2182929275	-1.152453298	1.1317123293
C 0.7797470719	-1.6293088795	0.377850302
C 1.1305097346	-0.9934641003	-0.8888225688
C 0.5453081013	0.1551146309	-1.2817789694
C -0.4700375262	0.8190585482	-0.4691757034
C -0.8741614044	2.0698185677	-0.7412955255
H -1.2714346005	0.6776881995	1.532852033
H -2.0372637019	-0.3774681303	0.3746530028
H -0.482522034	-1.6295597223	2.0699608786
H 1.3479520826	-2.4956813488	0.6989368234
H 1.9046880371	-1.4458686543	-1.4990592357
H 0.8557843133	0.6454232331	-2.1990489891
H -0.4877843675	2.6104225216	-1.5982119705
H -1.5999991278	2.5848340673	-0.1216345389
Core RigidRotor		
SymmetryFactor 1		
End		
Frequencies[1/cm] 39		
75.1688	267.6883	379.1625
439.6787	482.3186	550.2962
595.0901	662.0020	748.9726
765.4101	821.0622	887.5396
925.3781	947.5501	956.0485
980.5943	986.4939	996.2456
1025.9275	1180.3006	1200.7473
1222.0001	1311.4532	1336.4134

```

1394.0659          1430.0685          1451.4077
1466.6361          1615.9237          1660.1092
1704.7244          2961.3972          3043.7793
3131.7113          3151.3837          3156.4879
3171.5959          3182.6649          3213.9013
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
Fragment      H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]    1
0  2
End
GroundEnergy[kcal/mol] 26.29
End
!-----c2h3_c5h6_R6-1_p7-----
Bimolecular      R6-1_p7
Fragment      c5h6
RRHO
Geometry[angstrom]      11
C  1.7739473074      -0.6818466093      -0.7221071247
C  0.7200203695      -1.0943582551      -1.4506225047
C  -0.2941048379      -0.0324120696      -1.4821037331
C  0.1452095209      1.0236956202      -0.7726629161
C  1.5088975741      0.7111879701      -0.2184053795
H  2.6777413601      -1.2383555006      -0.515109658
H  0.6186967493      -2.0533819236      -1.9425843223
H  -1.2418186269      -0.1051309279      -2.0003409082
H  -0.3745603273      1.9578940938      -0.609861296
H  2.2675009981      1.4252972695      -0.5668910274
H  1.5278529127      0.7618083327      0.87884187
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]      27
348.5708          524.1051          681.3317
711.8753          817.0247          818.8020
917.6681          924.4172          953.9591
955.9506          970.7216          1012.6714
1112.1153         1124.7078          1130.0719
1265.2943         1314.9663          1397.2719
1414.9257         1551.9926          1639.1108
3009.5972         3031.2355          3186.6692
3196.7126         3215.2104          3221.8506
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
Fragment      c2h3
RRHO

```

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Geometry[angstrom] 5
C -2.6815309499 -1.8887734891 -1.1309235268
C -1.725733176 -1.3518528792 -0.4241833636
H -3.0692157655 -1.4200651964 -2.0332260024
H -3.1437000229 -2.8401606701 -0.8523521394
H -1.1628990858 -1.5707617651 0.4715150322
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 9
712.2118 819.4319 921.7170
1046.2369 1391.3607 1651.0507
3037.2336 3133.0072 3234.0563
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 34.89
End
!-----h_c7h8_R6-1_p8-----
Bimolecular R6-1_p8
Fragment c7h8
RRHO
Geometry[angstrom] 15
C -1.1387394626 0.5484523036 0.8328222671
C -0.844152618 0.0605040142 2.0335482956
C 1.7059527063 -0.4483363452 -1.0088575696
C 0.5941042962 -0.7944412163 -1.9045636258
C -0.5073287144 -0.1259652301 -1.5227003645
C -0.1785624065 0.7377859162 -0.3192625236
C 1.2755724215 0.4207379946 -0.0772038168
H -2.1649726202 0.8425447051 0.6201900591
H -1.6090387703 -0.0480747702 2.7943367618
H 0.1592582379 -0.2533405161 2.2974479904
H 2.7123138992 -0.8362932895 -1.103839341
H 0.6682948401 -1.4810713079 -2.738287987
H -1.4890931431 -0.1705592557 -1.9741505471
H -0.2486726719 1.7925532703 -0.6395888909
H 1.8626278124 0.8680606726 0.7130308765
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 39
90.5599 161.9479 237.9642
410.2024 529.4092 597.4855
633.0836 703.1293 729.0469
815.6273 843.5555 888.2748
946.2911 953.4842 961.6167
987.6759 1008.7959 1020.1425
1036.5893 1088.7096 1111.0904
1130.3752 1209.5174 1273.7542
1310.8948 1334.6368 1400.1563

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1446.7025          1556.9161          1640.9280
1703.5224          2948.9215          3120.5386
3138.6699          3185.8293          3196.1019
3214.8998          3218.2810          3221.4115
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0  1
End
Fragment            H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]    1
0  2
End
GroundEnergy[kcal/mol] 36.09
End
!-----h_c7h8_R6-1_p10-----
Bimolecular      R6-1_p10
Fragment          c7h8
RRHO
Geometry[angstrom]    15
C  -1.5859253695    0.3603087539    0.6031861375
C  -0.3170806041    0.0316385649    1.0746822957
C   0.7733581132   -0.0634901389    0.2037435599
C   0.5546998392    0.1751408462   -1.1570959493
C  -0.7121130138    0.5041455052   -1.6337938534
C  -1.788343386     0.5989274878   -0.7543188476
C   2.154062483    -0.3886604541    0.7221680017
H  -2.4175241098    0.4261346268    1.2963227141
H  -0.1706849106   -0.1561239174    2.1338552086
H   2.6973119257    0.5234725223    0.9930227207
H   1.3859872864    0.1001172192   -1.8512618829
H  -0.8590336601    0.6826750629   -2.6934491487
H  -2.7757242043    0.8519566561   -1.1237413162
H   2.7495900587   -0.9116551661   -0.0297820897
H   2.1073245508   -1.017377569    1.6144324525
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  39
25.2791          208.3916          343.7877
415.2520          476.5453          529.2377
637.7431          713.6407          744.5489
798.9305          855.0919          910.5769
975.7862          999.1745         1000.8220
1017.9113         1051.4699         1062.6347
1111.5615         1180.9829         1203.1449
1228.9765         1327.9160         1355.9448
1414.7593         1470.4004         1491.3629
1503.9825         1529.6569         1626.8235
1648.8606         3020.1450         3074.4788
3100.6412         3150.9983         3152.6365

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3165.2227          3173.5642          3186.3301
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]      1
0  1
End
Fragment          H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]      1
0  2
End
GroundEnergy[kcal/mol] -4.4
End
!-----ch3_c6h6_R6-1_p11-----
Bimolecular      R6-1_p11
Fragment          c6h6
RRHO
Geometry[angstrom]      12
C  1.0E-10      1.3939270249      0.0
C  1.2071772356      0.6969636998      0.0
C  1.2071772355      -0.6969636999      0.0
C  -1.0E-10      -1.3939270249      0.0
C  -1.2071772356      -0.6969636998      0.0
C  -1.2071772355      0.6969636999      0.0
H  1.0E-10      2.4783497639      0.0
H  2.1463150535      1.2391761454      0.0
H  2.1463150533      -1.2391761456      0.0
H  -1.0E-10      -2.4783497639      0.0
H  -2.1463150535      -1.2391761454      0.0
H  -2.1463150533      1.2391761456      0.0
Core RigidRotor
SymmetryFactor 12
End
Frequencies[1/cm]      30
412.8673          412.9205          623.1697
623.1905          688.6334          723.3029
862.2492          862.2578          981.2033
981.2120          1013.0553          1016.3126
1023.3089          1060.0803          1060.1305
1174.4625          1197.3620          1197.3631
1334.7654          1381.5716          1512.7366
1512.7704          1637.1235          1637.1258
3154.3644          3163.9812          3164.0151
3179.7630          3179.8002          3190.3895
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]      1
0  1
End
Fragment          ch3
RRHO
Geometry[angstrom]      4
C  0.0      1.995E-7      0.0

```

```

H 0.0 1.0804553795 0.0
H 0.9357017515 -0.5402277895 0.0
H -0.9357017515 -0.5402277895 0.0
Core RigidRotor
SymmetryFactor 6
End
Frequencies[1/cm] 6
505.1501 1403.0831 1403.0885
3103.6402 3282.6573 3282.6683
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -12.26
End
!-----c2h2_c5h7_R6-1_p13-----
Bimolecular R6-1_p13
Fragment c5h7
RRHO
Geometry[angstrom] 12
C -0.7686459253 0.7386317605 1.345063937
C -0.3071439945 -0.698802104 1.2316342677
C 0.9127876852 -0.5782823286 0.367527076
C 0.0238334462 1.5740307415 0.6747219123
C 1.1630248776 0.8509891718 -0.0119514018
H -1.6454139401 1.0293837496 1.9118058232
H -1.0831667091 -1.3468359608 0.7914580948
H -0.092627787 -1.1414306415 2.2185360959
H 1.5299289973 -1.4113325562 0.0589419032
H -0.1102725136 2.6476663443 0.6132612003
H 1.1559504298 1.0135488827 -1.1025652053
H 2.1465370552 1.2190043599 0.3244725608
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 30
206.9353 331.8221 391.3577
682.4467 742.4034 792.0774
896.7543 913.1768 924.2247
944.4211 961.6053 969.7489
1033.9880 1127.9478 1128.8759
1131.6486 1274.2401 1299.2586
1324.2372 1386.7572 1457.1040
1462.9995 1674.7401 2941.4534
2942.0039 2942.4294 2946.3936
3172.1535 3196.4215 3203.9815
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment c2h2
RRHO

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```

Geometry[angstrom] 4
C 0.0 0.0 0.5990703976
C 0.0 0.0 -0.5990703976
H 0.0 0.0 1.6619081422
H 0.0 0.0 -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 7
642.0679 642.0679 772.6955
772.6955 2069.5209 3420.9272
3523.7963
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 40.3
End
!-----R6-1_ts5-----
Barrier ts5 r1 ip4
RRHO
Geometry[angstrom] 16
C -0.9451499576 0.5918561912 0.8181330559
C -0.3179412784 -0.7515507444 1.1090525013
C 0.8717420031 -0.8346258916 0.1011741184
C 0.265213149 -0.9185994286 -1.2914288613
C -0.4315044913 0.1894579397 -1.5462875102
C -0.5225908566 1.1417313813 -0.3920255461
C 1.5272519893 0.5382599969 0.1327962489
H -1.3687028256 1.1997163202 1.6088841534
H -1.005374079 -1.5985275527 0.9856343719
H 0.04421986 -0.7795172924 2.1430668342
H 1.5492108979 -1.662531618 0.3333652366
H 0.3697522095 -1.7703751685 -1.9514170597
H -0.9793126848 0.3915070274 -2.4599979802
H -0.7116708555 2.1901681529 -0.6040482904
H 2.1608129278 0.8162050454 -0.7032350605
H 1.816376992 0.9549106413 1.095846788
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 611.583
WellDepth[kcal/mol] 26.53
WellDepth[kcal/mol] 25.1
End
Frequencies[1/cm] 41
306.2436 381.9325
397.9184 498.4337 580.8596
616.6099 653.2183 682.1464
718.0451 804.3179 840.6796
858.8884 901.6874 933.0261

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941.8577          953.9312          971.5149
978.5502          1021.5367         1069.7005
1119.3614         1128.6927         1158.3971
1213.9540         1288.0164         1306.0078
1348.9177         1378.8757         1416.6065
1453.1255         1471.2211         1657.8965
3001.3178         3035.5647         3041.2519
3091.7688         3147.9617         3169.1939
3179.5175         3195.6715         3200.3501
ZeroEnergy[kcal/mol] 26.53
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R6-1_ts6-----
Barrier          ts6  ip4  R6-1_p5
RRHO
Geometry[angstrom] 16
C -0.59325069  0.4765286331  1.5682983837
C -0.5836450635 -0.9934724875  1.2412400614
C 0.3305603415 -1.5055656445  0.4048231296
C 1.2815413509 -0.6384534481 -0.2792570355
C 1.1448730381 0.7020539897 -0.2552062832
C 0.0629319649 1.3421710859 0.500530405
C -0.1228759258 2.6914206302 0.4685456037
H -0.0214805696 0.6136357337 2.5013469422
H -1.6043876485 0.8296494739 1.7810584964
H -1.2914243225 -1.6353476918 1.7547976377
H 0.3698041623 -2.5726430886 0.2149010923
H 2.0754809739 -1.0933975811 -0.8614591606
H 1.8069487885 1.339140129 -0.8322689607
H -1.3076700702 0.8800309672 -0.7820164887
H 0.4572932506 3.3200030782 -0.1969475093
H -0.8910335804 3.1717462207 1.062988686
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling          Eckart
ImaginaryFrequency[1/cm] 752.4871
WellDepth[kcal/mol] 31.07
WellDepth[kcal/mol] 6.21
End
Frequencies[1/cm] 41
127.7275          287.2667
353.4778          408.0363          452.6230
472.4185          499.0491          549.4257
599.6797          623.1655          731.4014
766.2879          806.7236          852.9903
920.4425          940.3430          958.5433
981.7556          989.1097          993.5463
1026.0584         1175.9122         1198.5694
1216.4567         1306.5746         1325.8454

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1384.3676          1423.4891          1452.3467
1464.1621          1571.4339          1603.0558
1694.1447          2951.9266          3076.6670
3136.9906          3155.2578          3161.3118
3175.3637          3185.0628          3226.0279
ZeroEnergy[kcal/mol] 32.50
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R6-1_ts7-----
Barrier      ts7  r1  ip6
RRHO
Geometry[angstrom] 16
C -0.9852335998    0.4688946083    0.7884542047
C -0.4299727355   -0.6390008572    1.4333110452
C 1.0234259008   -0.8890519054   -0.1601496266
C 0.2399856706   -0.8990410759   -1.3793754047
C -0.373444235    0.3032671411   -1.5063452224
C -0.0668967177    1.1225330635   -0.2516175741
C 1.3407760331    0.5778741713    0.0816711791
H -2.05495914     0.5413465106    0.6180404821
H -1.0863804937   -1.44849764     1.7460945559
H 0.4480131378    -0.5401089338    2.0618323014
H 1.6905638185    -1.6926929671    0.1285815186
H 0.0875485692    -1.7657005941    -2.009611607
H -1.1013077849    0.590910076     -2.2537035384
H -0.1717604592    2.2026726742    -0.359735445
H 2.0735995991     0.9445175046    -0.6452015244
H 1.6883754365     0.8201632238    1.0872676554
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 695.1323
WellDepth[kcal/mol] 27.49
WellDepth[kcal/mol] 33.47
End
Frequencies[1/cm] 41
324.9445          372.7036
484.8636          497.8631          585.6661
662.2488          721.0624          726.5206
766.7670          794.2477          859.1094
881.2484          909.0995          914.7052
921.8648          945.1735          976.2590
1012.5187         1032.2726         1051.1578
1111.7372         1143.5790         1212.7831
1223.6896         1231.7314         1282.5352
1309.1338         1368.1864         1372.5013
1488.5260         1517.4155         1548.9815
3031.2948         3088.8393         3091.6877
3103.8127         3148.9068         3170.4112

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3178.1017          3191.1172          3211.8769
ZeroEnergy[kcal/mol] 27.49
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R6-1_ts8-----
Barrier          ts8 ip6 R6-1_p7
RRHO
Geometry[angstrom] 16
C -1.2054862971 0.5923700955 1.4085839747
C -1.4086185274 -0.6623418382 1.7236262835
C 1.7660997395 -0.6849344351 -0.7060155241
C 0.7167916988 -1.0878865936 -1.4573957091
C -0.2935787681 -0.0416234894 -1.4852548592
C 0.1074036274 0.9957670406 -0.695088099
C 1.5026358026 0.7044609299 -0.1929565358
H -1.4013046929 1.5256729726 1.9235276746
H -1.854579284 -0.959578775 2.676136111
H -1.1370593732 -1.4724336409 1.0494846412
H 2.6639498558 -1.2487361466 -0.4932391189
H 0.6299954319 -2.0377002956 -1.9700489321
H -1.2245662053 -0.0968461732 -2.0337732846
H -0.3565722113 1.9691431551 -0.6416196278
H 2.2180086201 1.4221915761 -0.6207405779
H 1.5992135833 0.780560618 0.8942865837
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 256.1294
WellDepth[kcal/mol] 43.03
WellDepth[kcal/mol] 2.16
End
Frequencies[1/cm] 41
42.1139          84.2214
124.0390         174.7433          258.4607
355.1152         516.9416          686.2089
742.2700         771.6862          811.0192
820.3543         866.2769          891.8190
910.4806         929.7259          934.8301
952.7684         973.1825         1026.6376
1070.4961        1106.0467         1122.7942
1130.3019        1270.6436         1313.1889
1388.9083        1393.6707         1419.1985
1476.8106        1594.9975         1643.0409
3001.7580        3045.0303         3065.3562
3133.1586        3185.8847         3188.1915
3203.2742        3218.0737         3229.8349
ZeroEnergy[kcal/mol] 37.05
ElectronicLevels[1/cm] 1
0 2

```

```

End
!-----
!-----R6-1_ts9-----
Barrier      ts9  ip6  R6-1_p8
RRHO
Geometry[angstrom]  16
C  -1.1573044531   0.5015245043   0.8563183447
C  -0.9033096761   0.1496124734   2.1118352274
C   1.7325727735  -0.4421744806  -1.0920022544
C   0.6154414862  -0.7542235614  -1.9775562805
C  -0.4991129633  -0.1559585908  -1.5151345992
C  -0.16446788   0.6413535857  -0.2719941461
C   1.2940872592   0.3135680457  -0.0546479278
H  -2.1812162008   0.7407742871   0.5743206143
H  -1.7013093585   0.0918445767   2.8436876537
H   0.0939347174  -0.1047023763   2.4510429377
H   2.7508702716  -0.7750076654  -1.245289339
H   0.6890092302  -1.3698219063  -2.864684387
H  -1.4908734282  -0.2021363879  -1.9440280043
H  -0.184775761   1.7050513629  -0.5785530263
H   1.9040177894   0.7728530786   0.7096067709
H   1.5247691938  -1.4144719456   1.3765914161
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  349.9455
WellDepth[kcal/mol]  45.65
WellDepth[kcal/mol]  3.58
End
Frequencies[1/cm]  41
85.5927          172.3085
209.5977          241.4124          368.4243
417.9879          530.2727          597.6694
619.2233          695.5232          756.2399
817.6190          844.1994          872.5552
948.2548          952.9856          957.2543
997.1182          1013.4770         1026.5038
1040.2943          1087.7966         1108.7725
1131.6803          1205.6356         1271.6509
1311.4827          1339.3034         1401.9782
1448.7328          1514.7366         1616.5779
1706.5110          2924.6491         3118.9954
3137.3346          3191.2760         3202.4527
3217.8885          3219.1062         3227.7904
ZeroEnergy[kcal/mol]  39.67
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----R6-1_ts10-----
Barrier      ts10  ip4  ip9

```

```

RRHO
Geometry[angstrom] 16
C -1.2573303295 0.5823666029 0.6612500801
C -0.2088756702 -0.3164261988 1.0951552525
C 0.7633870011 -0.9020182022 0.0412426354
C 0.4378450285 -0.5202801269 -1.3753374459
C -0.5311001713 0.3664032693 -1.6691779352
C -1.3814666458 0.9433054922 -0.6430425256
C 1.9534074039 -0.1580135849 0.6564871987
H -1.9163784582 1.0024248585 1.4140516672
H -0.4187529879 -0.9669541199 1.94234506
H 0.8529117607 0.3391699778 1.5539821797
H 0.8815235215 -1.9862361787 0.1226441318
H 1.0267934421 -0.9784976767 -2.1637119863
H -0.7160617972 0.64091987 -2.7026918527
H -2.152891162 1.6443171377 -0.9414615976
H 2.3172487241 0.7224263485 0.1363610441
H 2.67207334 -0.7148224691 1.2514170938
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1985.3523
WellDepth[kcal/mol] 30.07
WellDepth[kcal/mol] 54.2
End
Frequencies[1/cm] 41
126.5469 257.8094
357.9186 457.7279 528.5544
551.4809 583.8073 632.8270
705.2708 777.7237 804.5900
878.4203 884.7719 925.8442
957.2643 973.2238 982.2453
983.8248 1038.4819 1060.5364
1124.6714 1176.5495 1194.6845
1252.2720 1308.4612 1332.3764
1346.7049 1404.2582 1419.1666
1453.7591 1535.6160 1663.4001
1744.4180 3038.5581 3098.2577
3114.8087 3146.5265 3155.7565
3166.7747 3180.9484 3215.4490
ZeroEnergy[kcal/mol] 31.5
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R6-1_ts11-----
Barrier ts11 ip9 R6-1_p10
RRHO
Geometry[angstrom] 16
C -1.5819110933 0.364005486 0.6092938853
C -0.3341529258 -0.0207867189 1.0754708209

```

```

C 0.749846088 -0.2156025206 0.1847786104
C 0.5449407439 0.1239194456 -1.175029573
C -0.7051933516 0.5083205422 -1.635124085
C -1.779435329 0.6189034429 -0.749554542
C 2.1576101061 -0.3793034725 0.7241554964
H -2.4057772687 0.474531284 1.3058012053
H -0.1855982919 -0.213254199 2.1327967424
H 2.5848919314 0.6026899915 0.9542027796
H 0.5264283732 -2.0191284153 -0.0184585582
H 1.376774405 0.043925407 -1.8669139773
H -0.846086141 0.7312694602 -2.6870446505
H -2.7561090941 0.9183563542 -1.1118095583
H 2.8090065093 -0.8670491508 -0.0031770389
H 2.1670973394 -0.9727129364 1.6401254407
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 832.7005
WellDepth[kcal/mol] 25.54
WellDepth[kcal/mol] 7.24
End
Frequencies[1/cm] 41
176.8508 195.4447
321.7397 401.4129 443.2216
471.5203 507.4314 569.3044
630.8287 695.4786 746.4878
798.3179 842.3371 909.9103
976.1971 996.7380 998.9261
1007.8404 1043.5462 1062.8376
1116.0835 1178.6560 1198.7137
1216.2277 1315.7780 1353.7900
1415.2715 1467.2122 1491.5215
1503.8994 1510.9823 1597.0479
1627.1531 3024.8675 3086.7493
3113.8561 3156.6505 3159.7038
3170.8109 3176.8937 3189.2690
ZeroEnergy[kcal/mol] 2.84
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R6-1_ts12-----
Barrier ts12 ip9 R6-1_p11
RRHO
Geometry[angstrom] 16
C -1.4840111082 0.3686421817 0.6522716058
C -0.5628348654 -0.6182129877 0.9571340939
C 0.4345757846 -0.9883941531 0.012032256
C 0.3225044711 -0.4727111317 -1.3095541415
C -0.6043518653 0.5132105373 -1.5998741855
C -1.5000031725 0.9570174823 -0.6187107804

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```

C 2.2149854243 0.0290458346 0.772748287
H -2.2122368221 0.6746090241 1.3958069884
H -0.567990565 -1.0860795918 1.9353664851
H 1.8957669164 1.0622911644 0.7143911717
H 0.9715721614 -1.91783505 0.1621140478
H 0.9996506279 -0.8284442501 -2.0781836899
H -0.651591716 0.9310945881 -2.5998314749
H -2.2259726758 1.7269893175 -0.8528395895
H 2.9796735885 -0.2717541005 0.064378329
H 2.3125948197 -0.3813858643 1.7722655875
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 506.1388
WellDepth[kcal/mol] 22.12
WellDepth[kcal/mol] 11.68
End
Frequencies[1/cm] 41
115.8413 124.9686
165.9513 389.8749 417.7976
566.2482 567.3152 617.0388
627.1692 676.6024 718.2646
830.7260 862.7407 883.1482
972.5873 978.2642 980.9871
1003.3541 1029.4042 1042.3276
1051.4411 1171.1723 1176.5170
1194.0929 1323.3961 1375.2236
1424.2688 1426.6078 1485.7783
1500.8070 1577.3701 1603.7723
3072.8488 3152.7230 3161.3368
3161.4967 3177.7511 3178.4005
3189.6275 3219.6875 3236.1877
ZeroEnergy[kcal/mol] -0.58
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R6-1_ts13-----
Barrier ts13 r1 ip12
RRHO
Geometry[angstrom] 16
C -0.8709621033 0.6204536869 0.8956626324
C -0.277071382 -0.7465708669 1.149562081
C 0.8487797641 -0.7921349924 0.0656063318
C 0.1762025596 -0.9817353589 -1.2919773265
C -0.4294399292 0.0763714307 -1.7853798315
C -0.0475244424 1.3386277796 0.0673042279
C 1.3241371732 0.6749029998 0.0604643883
H -1.8667513823 0.9141362437 1.2014667956
H -1.0043306547 -1.5576403489 1.0409038135
H 0.1500078026 -0.8281280684 2.160171237

```

```

H  1.6235028451   -1.5317019175   0.2742598776
H  0.1736433541   -1.9660069144   -1.7619028016
H  -1.0731934025    0.2639554712   -2.6346740443
H  -0.2191333675    2.3645513335   -0.2329578689
H  1.9390993105    0.920210759   -0.8042637822
H  1.8753668546    0.9287937628    0.9752672698
Core RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  470.1445
WellDepth[kcal/mol]  29.6
WellDepth[kcal/mol]  10.4
End
Frequencies[1/cm]  41
284.4743          327.2255
375.9770          470.0882          531.5170
651.7478          678.7127          761.1993
778.7994          841.4270          860.5816
865.8655          892.7175          911.2320
933.5745          960.8556          965.5837
1020.9592         1025.9098         1098.0371
1145.9984         1152.9091         1199.8444
1216.8177         1286.6403         1293.1231
1322.8675         1357.3821         1464.1559
1481.2480         1498.4654         1633.0746
2976.9041         3006.2260         3045.1222
3078.5447         3091.1797         3112.1549
3186.9973         3205.4429         3207.7567
ZeroEnergy[kcal/mol]  29.6
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----R6-1_ts14-----
Barrier      ts14  ip12  R6-1_p13
RRHO
Geometry[angstrom]  16
C  -0.7792839672    0.736480118    1.3289000473
C  -0.3217976772   -0.7000492916    1.2037728498
C  0.7986560008   -0.6077997885    0.1893358671
C  -0.1422805424   -1.3677449649   -1.7030637645
C  -0.0855371425   -0.6633518439   -2.7019105499
C  0.0149315332    1.5711386951    0.6612747163
C  1.1451005899    0.8450906734   -0.0333853149
H  -1.6471732842    1.0265957261    1.9093223071
H  -1.134085506    -1.3750983122    0.8986667101
H  0.0346212179    -1.0914721598    2.1704957742
H  1.5789629148    -1.3605060982    0.1681241588
H  -0.4540372778   -2.2654456911   -1.2119892968
H  0.0793963413    0.0980560804   -3.4264296527
H  -0.1076079777    2.6469890309    0.6154419148

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H 1.2227224961 1.100234241 -1.0982679283
H 2.1197452813 1.104968585 0.4092251618
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 492.0794
WellDepth[kcal/mol] 29.2
WellDepth[kcal/mol] 8.1
End
Frequencies[1/cm] 41
28.4087 87.7890
176.8984 250.8191 324.5303
393.0073 502.3501 633.2994
681.1427 705.3190 760.6337
762.3618 791.8422 817.3479
895.9891 917.9895 923.7294
967.5550 969.8653 988.9536
1047.6548 1128.3443 1150.2613
1168.7619 1267.3452 1301.4375
1326.1841 1380.8495 1460.9865
1468.2672 1677.6780 1882.9387
2952.8546 2961.8289 2981.6921
3003.1147 3165.0944 3172.0195
3196.5910 3339.1200 3458.9427
ZeroEnergy[kcal/mol] 48.4
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```

R6_secondary_c7h9-7

```
Well          r7
Species
RRHO
Geometry[angstrom]  16
C  -1.1084819087    0.501792809    0.7744168792
C  -0.3833197226    -0.8416928474    1.1067688844
C   0.8510134286    -0.8271601871    0.1165537225
C   0.2528277766    -0.9582093595    -1.2815834556
C  -0.3678197149    0.19164514    -1.5660349097
C  -0.1987971121    1.1177914806    -0.3645891789
C   1.1550721829    0.6541252222    0.1240475788
H  -1.1283388014    1.165962337    1.6421888905
H  -2.1375679011    0.3604980425    0.4364616192
H  -1.0151128401    -1.7190398916    0.9508985236
H  -0.035855911    -0.8580470794    2.1428891285
H   1.646575768    -1.522975978    0.3775988962
H   0.2505127574    -1.8689075574    -1.86729837
H  -0.980360248    0.4114929642    -2.4314247395
H  -0.3528741392    2.1813433073    -0.5387770519
H   1.7694003894    1.1670526028    0.8570745789
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  42
246.5264          348.4458          376.0452
479.1601          666.4217          675.6893
722.7455          782.4872          801.1710
819.2789          829.0853          853.7848
905.4055          926.0791          947.5726
949.8077          961.9588          974.9799
1052.7132         1109.5746         1137.1793
1158.2960         1180.6188         1220.3579
1233.9259         1280.6717         1284.2909
1304.6213         1315.7509         1355.3018
1488.1330         1503.8778         1632.2664
3037.7433         3048.6271         3075.4531
3093.1464         3111.7244         3112.9195
3166.4947         3182.2071         3207.2373
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----R6-1_ip14-----
Well          ip14
Species
RRHO
Geometry[angstrom]  16
```

```

C  -1.1817270214    0.6772468016    0.9798794394
C  -1.2975012492   -0.6606923529    1.6231479423
C   1.6870583554   -0.5940239491   -0.6676790606
C   0.6150156652   -0.9416014236   -1.6115330998
C  -0.4705489818   -0.1937517431   -1.3427463478
C  -0.172460798    0.7342931823   -0.1899216732
C   1.2464501823    0.3630298043    0.1684889215
H  -0.8998375114    1.4350567614    1.7260854006
H  -2.1640335747    1.0104296249    0.6059732262
H  -0.820016908    -1.5314439174    1.1938420085
H  -1.9067322649   -0.7884933377    2.5095455865
H   2.670542682   -1.046833983   -0.6627088032
H   0.7047287906   -1.6826705428   -2.3958700708
H  -1.4200952395   -0.2174038445   -1.8611252864
H  -0.1730344089    1.7676546928   -0.572076266
H   1.7992777892    0.8249671115    0.975799008
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 42
56.4111          127.6664          130.9545
286.6952          333.4419          442.4976
554.2679          581.0287          703.0222
721.1213          809.6154          832.5353
872.3102          873.1358          939.5011
955.9131          956.4258         1002.6222
1027.7303         1042.2267         1093.7332
1110.6941         1148.0062         1161.5957
1249.1715         1277.8731         1319.2338
1362.8964         1402.0091         1458.2424
1467.2157         1554.0887         1638.7439
2941.6420         2971.6652         2981.1583
3142.0621         3183.5559         3192.7657
3209.5230         3216.9951         3248.0024
ZeroEnergy[kcal/mol] -2.6
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----R6-1_ip16-----
Well      ip16
Species
RRHO
Geometry[angstrom] 16
C  -1.1336676812    0.3403404695    0.7584462376
C  -0.4117775449   -0.7709835012    1.5610994556
C   1.0428015349   -0.5491228515    1.2202762531
C   0.2233483647   -0.6780171339   -2.3837503991
C  -0.459570921    0.2168852048   -1.7178680962
C  -0.123075934    0.7828433213   -0.3480444419
C   1.1997705826    0.2875719744    0.1978346387

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H -1.3367210139    1.1900353062    1.4152996164
H -2.0880109267    0.0116575358    0.3421110233
H -0.7283491266   -1.7749773564    1.2515944065
H -0.613121968    -0.6992967127    2.6346041057
H  1.8501974008   -1.0564811135    1.7364371377
H  0.1599963719   -1.1985572132   -3.327461132
H -1.379249786    0.6156904374   -2.16621349
H -0.133062962    1.8758105134   -0.4452810155
H  2.1474668084    0.5623629171   -0.2497427254
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  42
72.9218            122.8650            199.8167
330.9036            382.7900            541.2271
620.3780            689.4139            728.6850
779.3762            790.2030            838.0120
848.3259            882.8399            917.6275
957.6688            973.6244           1015.7600
1047.8895           1079.3199           1133.0915
1176.8209           1217.1873           1243.5562
1269.0661           1313.2004           1325.7471
1332.7251           1381.6656           1483.5852
1500.9908           1665.4581           1683.0665
2993.6181           3004.6807           3008.3151
3039.9517           3053.5466           3090.5155
3169.3657           3195.5544           3239.0865
ZeroEnergy[kcal/mol] 12.9
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----c2h4_c5h5_R6-1_p15-----
Bimolecular R6-1_p15
Fragment c5h5
RRHO
Geometry[angstrom] 10
C 0.0 0.741277 -0.946378
C 0.0 1.169009 0.352883
C 0.0 0.0 1.186344
C 0.0 -1.169009 0.352883
C 0.0 -0.741277 -0.946378
H 0.0 1.357995 -1.834653
H 0.0 2.190729 0.702061
H 0.0 0.0 2.269063
H 0.0 -2.190729 0.702061
H 0.0 -1.357995 -1.834653
Core RigidRotor
SymmetryFactor 10
End
Frequencies[1/cm] 24

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79.4819          499.9744          515.7639
681.0549          718.8982          815.8713
847.4073          891.7157          898.7753
928.9567          944.2116        1059.0104
1072.5562         1143.4061         1216.8702
1295.0222         1386.6341         1490.4168
1534.4297         3198.9889         3204.2383
3215.6789         3231.0539         3239.2445
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment          c2h4
RRHO
Geometry[angstrom] 6
C 0.0 0.6634900906 0.0
C 0.0 -0.6634900906 0.0
H 0.0 1.23462754 -0.9225248038
H 0.0 1.23462754 0.9225248038
H 0.0 -1.23462754 0.9225248038
H 0.0 -1.23462754 -0.9225248038
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm] 12
834.2929          972.9227          974.1218
1066.8559         1238.5875         1379.4650
1472.0483         1691.5384         3121.2072
3136.3255         3192.3844         3220.8390
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 2.5
End
!-----c2h2_c5h7_R6-1_p17-----
Bimolecular      R6-1_p17
Fragment          c5h7
RRHO
Geometry[angstrom] 12
C -1.1010414736 0.3918722625 0.8234640968
C -0.3631520631 -0.8239462751 1.462982238
C 1.0707741887 -0.6501660094 1.0310183231
C -0.0133737739 1.136197524 0.0914150965
C 1.202988679 0.4885220714 0.2499527768
H -1.583484021 1.0209968724 1.5815071743
H -1.9013102667 0.0723672176 0.1447410417
H -0.777380506 -1.7795464887 1.118858777
H -0.4595285948 -0.8309072566 2.5556128554
H 1.8692946452 -1.3279976329 1.3019040122
H -0.1777388973 2.0449229769 -0.4722088268
H 2.1372330834 0.8286777379 -0.1813115651

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Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 30
123.2749          449.8385          597.4547
642.6361          726.9177          803.1772
810.9431          905.7597          912.4748
947.4334          992.0506         1027.4342
1072.4356         1105.1135         1141.8722
1221.8220         1273.6993         1300.2750
1317.5741         1400.1897         1469.6527
1478.1960         1492.7815         2996.2094
3007.3562         3009.1704         3029.4467
3179.0296         3201.0085         3212.7167
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment          c2h2
RRHO
Geometry[angstrom] 4
C 0.0 0.0 0.5990703976
C 0.0 0.0 -0.5990703976
H 0.0 0.0 1.6619081422
H 0.0 0.0 -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 7
642.0679          642.0679          772.6955
772.6955          2069.5209         3420.9272
3523.7963
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 21.7
End
!-----R6-1_ts15-----
Barrier          ts15  r7  ip14
RRHO
Geometry[angstrom] 16
C -1.124062371 0.5347725873 0.8093524999
C -0.6137831133 -0.8183503857 1.2233121958
C 1.1482579584 -0.7547965642 -0.1078186066
C 0.3456202189 -0.9617953119 -1.3269125269
C -0.3967620222 0.1414582034 -1.5387552719
C -0.1666313659 1.0786885788 -0.3904945511
C 1.1634070018 0.6228627136 0.1500607066
H -1.0537528645 1.2481953786 1.6338594567
H -2.1609024193 0.5207650343 0.4688120068
H -1.120520468 -1.7054444068 0.8625138938

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H -0.1841436418 -0.9175141797 2.2140112043
H 1.8766282431 -1.4668222098 0.2587889529
H 0.3137995763 -1.8860110803 -1.8894117986
H -1.1594990305 0.2772930921 -2.2939434645
H -0.3250574394 2.1409496421 -0.5707625583
H 1.6744872442 1.1015117927 0.9764887864
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 534.2247
WellDepth[kcal/mol] 18.6
WellDepth[kcal/mol] 21.2
End
Frequencies[1/cm] 41
209.5208 315.1068
457.8574 494.6581 609.5539
624.2562 698.1247 725.2723
773.5261 804.6989 824.3910
837.4916 862.4743 920.8073
925.8101 954.1882 959.0617
997.8468 1025.2354 1057.7508
1082.5681 1126.1163 1131.4064
1229.5467 1280.0641 1287.9709
1310.0116 1372.9004 1397.6626
1466.7207 1505.1533 1600.5642
3047.5918 3090.3330 3110.8173
3127.5877 3181.5188 3189.8963
3201.6177 3215.2724 3216.3725
ZeroEnergy[kcal/mol] 18.6
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R6-1_ts16-----
Barrier ts16 ip14 R6-1_p15
RRHO
Geometry[angstrom] 16
C -1.4549413981 0.5725165228 1.0691794956
C -1.4668392941 -0.7434730613 1.4840203716
C 1.689428791 -0.6516178828 -0.4171683713
C 0.7234483965 -0.975204177 -1.4712914881
C -0.2501069628 -0.0278622982 -1.4794558384
C 0.0290378483 0.9149061737 -0.3958242461
C 1.2934784944 0.4892115737 0.2049776836
H -1.0472089431 1.3247449355 1.7356597906
H -2.2517141385 0.9212954622 0.4212629196
H -2.0332329013 -1.4961964736 0.9496503284
H -0.815991724 -1.0884833388 2.2779416752
H 2.5723516779 -1.2341443069 -0.1891876309
H 0.7930341702 -1.830184198 -2.1308611075
H -1.1033347023 0.0250366081 -2.1408502794

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H -0.252924571 1.9600936729 -0.4582815384
H 1.7926007638 0.9951236724 1.0193291606
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 556.2822
WellDepth[kcal/mol] 18.8
WellDepth[kcal/mol] 13.7
End
Frequencies[1/cm] 41
60.3922 113.2630
166.8638 281.8099 387.6325
559.6055 563.3441 715.3158
733.3348 768.3880 790.2167
815.0046 832.6049 857.3940
908.3937 921.3753 964.3869
964.9098 1019.5559 1019.5610
1050.7627 1098.8281 1141.4620
1245.4539 1249.7250 1279.7350
1307.8730 1395.3782 1467.6375
1505.9431 1545.7562 1581.1859
3119.7453 3144.1706 3168.2467
3191.5449 3197.7272 3202.3183
3218.0324 3225.7706 3238.6906
ZeroEnergy[kcal/mol] 16.2
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----R6-1_ts17-----
Barrier ts17 r7 ip16
RRHO
Geometry[angstrom] 16
C -1.1607711141 0.4656375719 0.8098030521
C -0.4558582542 -0.8657279056 1.2025445545
C 0.9445279853 -0.6946792386 0.6176212096
C 0.2742739302 -0.9299900764 -1.512201943
C -0.3567009569 0.2318364429 -1.5425428798
C -0.215765174 1.0679417501 -0.2668139495
C 1.142161543 0.6100527914 0.2306238113
H -1.213081939 1.1398417939 1.6696098817
H -2.1761471349 0.3137089598 0.4373197365
H -0.9676278782 -1.7482632543 0.815059072
H -0.4011321712 -0.9813552763 2.2903940058
H 1.7393348977 -1.4005538377 0.8290030623
H 0.3385007444 -1.7729605788 -2.1891175325
H -1.0002869662 0.5569459861 -2.360404186
H -0.3509499934 2.1388243477 -0.4244108588
H 2.0764956806 1.0245023211 -0.1271454618
Core RigidRotor
SymmetryFactor 0.5

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End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  527.8861
WellDepth[kcal/mol]  29.2
WellDepth[kcal/mol]  16.3
End
Frequencies[1/cm]  41
236.0114          289.5011
397.1125          484.1855          581.2630
654.6643          730.7028          752.1803
792.0753          825.5366          841.3248
877.5223          897.6684          902.5908
915.7620          948.8624          989.0110
1020.2898         1043.3756         1096.8378
1151.8345         1202.7242         1205.3920
1247.2931         1276.3642         1299.1035
1313.1857         1351.5728         1464.8560
1490.0620         1505.5962         1610.2088
3025.3626         3041.6829         3073.7582
3085.2600         3090.4950         3099.8127
3176.8197         3196.9516         3199.0051
ZeroEnergy[kcal/mol]  29.2
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----R6-1_ts18-----
Barrier      ts18  ip16  R6-1_p17
RRHO
Geometry[angstrom]  16
C  -1.1032386065   0.3887313559   0.824253303
C  -0.3770063258  -0.8486888207   1.4153404107
C   1.0739165682  -0.5828727196   1.0954345774
C  -0.1579917106  -0.8610268565  -2.4586705852
C  -0.6457533934   0.1958697608  -2.0450527207
C  -0.0820328001   0.9951126792  -0.1228103015
C   1.2034799701   0.4611065494   0.2458295305
H  -1.3285219577   1.1081648182   1.62284121
H  -2.0522786319   0.1384597504   0.3444044376
H  -0.7136869292  -1.7746886385   0.9313418324
H  -0.5615266074  -0.9742959044   2.4870829216
H   1.8885786334  -1.1823870229   1.4831725867
H   0.4713830626  -1.7221836963  -2.4636939432
H  -1.3539456085   0.9721099619  -2.2611764018
H  -0.186020199   2.02063175   -0.4607284618
H   2.1416177347   0.8217188306  -0.1582268212
Core  RigidRotor
SymmetryFactor  1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  618.9274
WellDepth[kcal/mol]  23.6

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WellDepth[kcal/mol]  14.8
End
Frequencies[1/cm]   41
38.7413              97.3221
151.3634             232.5605          300.3323
455.2678             537.1547          636.5950
691.9595             729.5864          753.4956
775.7337             810.8820          830.9951
892.1324             918.2728          926.3972
961.3643            1017.1426        1021.2858
1060.8500            1124.2209        1153.5563
1224.8168            1280.3324        1305.7633
1326.6317            1392.3088        1469.0572
1487.8599            1563.3827        1822.7721
2994.1715            3003.0417        3044.3930
3068.5451            3156.1519        3179.8596
3201.9376            3301.9695        3417.1562
ZeroEnergy[kcal/mol] 36.5
ElectronicLevels[1/cm] 1
0  2
End
!-----
End

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